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**Thermodynamic Properties
of Polycyclic Aromatic Hydrocarbons**

Thomas C. Allison
Donald R. Burgess Jr.

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*Material Measurement Laboratory
Chemical Sciences Division*

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National Institute of Standards and Technology
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3.274	Anthra[2,1,9,8- <i>opqra</i>]naphthacene	564
3.275	Dibenzo[<i>cd,lm</i>]perylene	566
3.276	Phenanthro[3,4- <i>c</i>]phenanthrene	568
3.277	Dibenzo[<i>g,p</i>]chrysene	570
3.278	Naphtho[2,3- <i>g</i>]chrysene	572
3.279	Phenanthro[4,3- <i>a</i>]anthracene	574
3.280	Naphtho[1,2- <i>g</i>]chrysene	576
3.281	Dibenzo[<i>c,p</i>]chrysene	578
3.282	Anthra[1,2- <i>a</i>]anthracene	580
3.283	Naphtho[2,1- <i>c</i>]chrysene	582
3.284	Benzo[<i>a</i>]naphth[2,1- <i>j</i>]anthracene	584
3.285	Dibenzo[<i>c,g</i>]chrysene	586
3.286	Benzo[<i>h</i>]pentaphene	588
3.287	Dibenzo[<i>a,c</i>]naphthacene	590
3.288	Naphtho[1,2- <i>b</i>]triphenylene	592

3.289	Dibenzo[<i>b,p</i>]chrysene	594
3.290	Naphtho[2,3- <i>c</i>]chrysene	596
3.291	Dibenzo[<i>a,c</i>]tetraphene	598
3.292	Benzo[<i>f</i>]picene	600
3.293	Benzo[<i>s</i>]picene	602
3.294	Benzo[<i>a</i>]pentaphene	604
3.295	Naphtho[1,2- <i>a</i>]naphthacene	606
3.296	Benzo[<i>a</i>]naphtho[1,2- <i>h</i>]anthracene	608
3.297	Benzo[<i>a</i>]picene	610
3.298	Dibenzo[<i>c,l</i>]chrysene	612
3.299	Naphtho[1,2- <i>c</i>]chrysene	614
3.300	Naphtho[2,1- <i>b</i>]chrysene	616
3.301	Dibenzo[<i>b,l</i>]chrysene	618
3.302	Dibenzo[<i>a,l</i>]naphthacene	620
3.303	Hexaphene	622
3.304	Benzo[<i>c</i>]pentaphene	624
3.305	Dibenzo[<i>a,j</i>]naphthacene	626
3.306	Benzo[<i>a</i>]pentacene	628
3.307	Benzo[<i>b</i>]picene	630
3.308	Naphtho[2,1- <i>a</i>]naphthacene	632
3.309	Naphtho[1,2- <i>b</i>]chrysene	634
3.310	Dibenzo[<i>b,k</i>]chrysene	636
3.311	Benzo[<i>c</i>]picene	638
3.312	Hexacene	640
3.313	8 <i>H</i> -Tribenzo[<i>a,cd,l</i>]pyrene	642
3.314	9 <i>H</i> -Naphtho[1,2,3- <i>cd</i>]perylene	644
3.315	Truxene	646
3.316	Diindeno[1,2,3- <i>cd:1',d',3'-jk</i>]pyrene	648
3.317	Acenaphtho[1,2- <i>k</i>]cyclopenta[<i>cd</i>]fluoranthene	650
3.318	Phenanthro[1,10,9,8- <i>opqra</i>]perylene	652
3.319	Benzo[<i>cd</i>]naphtho[3,2,1,8- <i>pqra</i>]perylene	654
3.320	Benzo[<i>a</i>]coronene	656
3.321	Phenanthro[5,4,3,2- <i>abcde</i>]perylene	658
3.322	Benzo[<i>lmn</i>]naphtho[2,1,8- <i>gra</i>]perylene	660
3.323	Benzo[<i>pqr</i>]naphtho[8,1,2- <i>bcd</i>]perylene	662
3.324	Phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene	664
3.325	peri-Naphthacenonaphthacene	666
3.326	Fluoreno[9,1- <i>ab</i>]triphenylene	668
3.327	Anthra[1,2- <i>a</i>]aceanthrylene	670
3.328	Anthra[2,1- <i>a</i>]aceanthrylene	672
3.329	Dibenzo[<i>a,o</i>]perylene	674
3.330	Phenanthro[1,2,3,4- <i>def</i>]chrysene	676
3.331	Benzo[<i>fg</i>]naphtho[1,2,3- <i>op</i>]naphthacene	678
3.332	Benzo[<i>p</i>]naphtho[1,8,7- <i>ghi</i>]chrysene	680
3.333	Dibenzo[<i>a,f</i>]perylene	682

3.334	Tribenzo[<i>c,g,mno</i>]chrysene	684
3.335	Dibenzo[<i>a,n</i>]perylene	686
3.336	Benzo[<i>de</i>]naphtho[3,2,1- <i>mn</i>]naphthacene	688
3.337	Benzo[<i>mno</i>]naphtho[2,1- <i>c</i>]chrysene	690
3.338	Benzo[<i>c</i>]naphtho[8,1,2- <i>ghi</i>]chrysene	692
3.339	Tribenzo[<i>b,def,p</i>]chrysene	694
3.340	Phenanthro[9,10,1- <i>gra</i>]naphthacene	696
3.341	Dibenzo[<i>h,rst</i>]pentaphene	698
3.342	Dibenzo[<i>a,j</i>]perylene	700
3.343	Naphtho[2,1,8- <i>fgh</i>]pentaphene	702
3.344	Naphtho[1,2- <i>b</i>]perylene	704
3.345	Naphtho[1,2,3,4- <i>rst</i>]pentaphene	706
3.346	Benzo[<i>a</i>]naphtho[8,1,2- <i>cde</i>]naphthacene	708
3.347	Dibenzo[<i>f,pqr</i>]picene	710
3.348	Benzo[<i>b</i>]naphtho[8,1,2- <i>pqr</i>]chrysene	712
3.349	Tribenzo[<i>a,hi,mn</i>]naphthacene	714
3.350	Dibenzo[<i>de,uv</i>]pentacene	716
3.351	Dibenzo[<i>pq,uv</i>]pentaphene	718
3.352	Dibenzo[<i>de,uv</i>]pentaphene	720
3.353	Dibenzo[<i>a,rst</i>]pentaphene	722
3.354	Naphtho[2,1,8- <i>uva</i>]pentaphene	724
3.355	Dibenzo[<i>de,ij</i>]pentaphene	726
3.356	Naphtho[2,1,8- <i>def</i>]picene	728
3.357	Dibenzo[<i>fg,ij</i>]pentaphene	730
3.358	Dibenzo[<i>de,st</i>]pentacene	732
3.359	Naphtho[2,1- <i>b</i>]perylene	734
3.360	Dibenzo[<i>a,pqr</i>]picene	736
3.361	Dibenzo[<i>fg,qr</i>]pentacene	738
3.362	Dibenzo[<i>de,qr</i>]pentacene	740
3.363	Dibenzo[<i>de,kl</i>]pentaphene	742
3.364	Benzo[<i>mno</i>]naphtho[1,2- <i>c</i>]chrysene	744
3.365	Benzo[<i>a</i>]naphtho[8,1,2- <i>lmn</i>]naphthacene	746
3.366	Benzo[<i>vwx</i>]hexaphene	748
3.367	Benzo[<i>a</i>]naphtho[2,1,8- <i>hij</i>]naphthacene	750
3.368	Naphtho[2,1,8- <i>uva</i>]pentacene	752
3.369	Anthra[2,1,9- <i>gra</i>]naphthacene	754
3.370	Naphtho[8,1,2- <i>cde</i>]pentaphene	756
3.371	Dibenzo[<i>c,pqr</i>]picene	758
3.372	Dibenzo[<i>c,rst</i>]pentaphene	760
3.373	Dibenzo[<i>b,tuv</i>]picene	762
3.374	1 <i>H</i> -Dibenzo[<i>a,de</i>]naphth[2,3- <i>h</i>]anthracene	764
3.375	4 <i>H</i> -Dibenzo[<i>a,de</i>]pentacene	766
3.376	Dicyclopenta[<i>a,j</i>]coronene	768
3.377	Dibenz[<i>e,ghi</i>]indeno[1,2,3,4- <i>pqra</i>]perylene	770
3.378	Dibenzo[<i>mn,qr</i>]fluoreno[2,1,9,8,7- <i>defghi</i>]naphthacene	772

3.379	Dibenzo[<i>bc,ef</i>]coronene	774
3.380	Naphtho[8,1,2- <i>abc</i>]coronene	776
3.381	Dibenzo[<i>bc,kl</i>]coronene	778
3.382	Naphth[1',2':5,6]indeno[1,2,3- <i>cd</i>]pyrene	780
3.383	Naphth[2',1':4,5]indeno[1,2,3- <i>cd</i>]pyrene	782
3.384	Tribenzo[<i>a,e,ghi</i>]perylene	784
3.385	Benzo[<i>a</i>]naphtho[2,1,8- <i>cde</i>]perylene	786
3.386	Dibenzo[<i>c,hi</i>]naphtho[3,2,1,8- <i>mnp</i>]chrysene	788
3.387	Benzo[<i>b</i>]naphtho[1,2,3,4- <i>pqr</i>]perylene	790
3.388	Tribenzo[<i>b,e,ghi</i>]perylene	792
3.389	Benzo[<i>h</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	794
3.390	Phenanthro[9,10,1,2,3- <i>pqrst</i>]pentaphene	796
3.391	Benzo[<i>a</i>]naphtho[2,1,8- <i>lmn</i>]perylene	798
3.392	Tetrabenzo[<i>de,hi,mn,qr</i>]naphthacene	800
3.393	Anthra[9,1,2- <i>bcd</i>]perylene	802
3.394	Benzo[<i>a</i>]naphtho[8,1,2- <i>klm</i>]perylene	804
3.395	Dibenzo[<i>de,mn</i>]naphtho[2,1,8- <i>gra</i>]naphthacene	806
3.396	Tribenzo[<i>a,cd,lm</i>]perylene	808
3.397	Phenanthro[1,2,3,4- <i>ghi</i>]perylene	810
3.398	Benzo[<i>pqr</i>]naphtho[1,2- <i>b</i>]perylene	812
3.399	Benzo[<i>lm</i>]naphtho[1,8- <i>ab</i>]perylene	814
3.400	Benzo[<i>rst</i>]naphtho[2,1,8- <i>fgh</i>]pentaphene	816
3.401	Benzo[<i>a</i>]naphtho[1,2,3,4- <i>ghi</i>]perylene	818
3.402	Benzo[<i>uv</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	820
3.403	Tribenzo[<i>a,ghi,k</i>]perylene	822
3.404	Anthra[2,1,9,8- <i>defgh</i>]pentaphene	824
3.405	Benzo[<i>ghi</i>]naphtho[2,1- <i>a</i>]perylene	826
3.406	Dibenzo[<i>b,qr</i>]naphtho[3,2,1,8- <i>defg</i>]chrysene	828
3.407	Anthra[8,9,1,2- <i>cdefg</i>]benzo[<i>a</i>]naphthacene	830
3.408	Benzo[<i>de</i>]naphtho[8,1,2,3- <i>stuv</i>]picene	832
3.409	Benzo[<i>ghi</i>]naphtho[2,1- <i>b</i>]perylene	834
3.410	Benzo[<i>uv</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene	836
3.411	Benzo[<i>pqr</i>]naphtho[2,1,8- <i>def</i>]picene	838
3.412	Benzo[<i>a</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	840
3.413	Benzo[<i>st</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene	842
3.414	Benzo[<i>qr</i>]naphtho[2,1,8,7- <i>fghi</i>]pentacene	844
3.415	Benzo[<i>pqr</i>]naphtho[2,1- <i>b</i>]perylene	846
3.416	Tribenzo[<i>b,n,pqr</i>]perylene	848
3.417	Benzo[<i>kl</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	850
3.418	Benzo[<i>ij</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene	852
3.419	Tribenzo[<i>de,ij,rst</i>]pentaphene	854
3.420	Benzo[<i>de</i>]naphtho[2,1,8,7- <i>qrst</i>]pentacene	856
3.421	Benzo[<i>qr</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene	858
3.422	Naphtho[3,2,1,8,7- <i>vwxyz</i>]hexaphene	860
3.423	Pyranthrene	862

3.424	Benzo[<i>c</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene	864
3.425	Phenanthro[2,3,4,5- <i>tuvab</i>]picene	866
3.426	Naphtho[7,8,1,2,3- <i>tuvwx</i>]hexaphene	868
3.427	Tribenzo[<i>de,kl,rst</i>]pentaphene	870
3.428	Anthra[8,9,1,2- <i>lmnop</i>]benzo[<i>a</i>]naphthacene	872
3.429	Dinaphtho[8,1,2- <i>lmn:2',1',8'-gra</i>]naphthacene	874
3.430	Anthra[2,1,9,8- <i>stuva</i>]pentacene	876
3.431	Naphthaceno[2,1,12,11- <i>opqra</i>]naphthacene	878
3.432	Benzo[<i>pqr</i>]naphtho[8,1,2- <i>cde</i>]picene	880
3.433	Benzo[<i>rst</i>]naphtho[8,1,2- <i>cde</i>]pentaphene	882
3.434	Benzo[<i>c</i>]naphtho[2,1- <i>p</i>]chrysene	884
3.435	Benzo[2,1- <i>a:3,4-a'</i>]dianthracene	886
3.436	Dinaphtho[2,1- <i>c 1',2'-g</i>]phenanthrene	888
3.437	Trinaphthylene	890
3.438	Anthra[1,2- <i>a</i>]benz[<i>j</i>]anthracene	892
3.439	Naphtho[1,2- <i>h</i>]pentaphene	894
3.440	Naphtho[2,3- <i>s</i>]picene	896
3.441	Phenanthro[3,2- <i>g</i>]chrysene	898
3.442	Dinaphth[1,2- <i>a:2',1'-j</i>]anthracene	900
3.443	Dibenzo[<i>a,h</i>]pentaphene	902
3.444	Benzo[<i>b</i>]naphtho[2,3- <i>g</i>]chrysene	904
3.445	Benzo[<i>b</i>]naphtho[2,1- <i>p</i>]chrysene	906
3.446	Phenanthro[9,10- <i>b</i>]triphenylene	908
3.447	Tribenzo[<i>b,g,p</i>]chrysene	910
3.448	Dibenzo[<i>f,s</i>]picene	912
3.449	Phenanthro[3,4- <i>c</i>]chrysene	914
3.450	Phenanthro[2,3- <i>g</i>]chrysene	916
3.451	Dibenzo[<i>a,f</i>]picene	918
3.452	Anthra[1,2- <i>a</i>]naphthacene	920
3.453	Naphtho[1,2- <i>a</i>]pentaphene	922
3.454	Benzo[<i>b</i>]naphtho[2,1- <i>g</i>]chrysene	924
3.455	Phenanthro[2,3- <i>c</i>]chrysene	926
3.456	Dibenzo[<i>a,o</i>]pentaphene	928
3.457	Naphtho[1,2- <i>f</i>]picene	930
3.458	Phenanthro[3,4- <i>b</i>]triphenylene	932
3.459	Dibenzo[<i>a,j</i>]picene	934
3.460	Tribenzo[<i>b,g,l</i>]chrysene	936
3.461	Benzo[<i>a</i>]naphtho[2,1- <i>l</i>]naphthacene	938
3.462	Naphtho[2,3- <i>a</i>]picene	940
3.463	Naphtho[2,3- <i>a</i>]pentaphene	942
3.464	Phenanthro[3,4- <i>b</i>]chrysene	944
3.465	Benzo[<i>g</i>]naphtho[2,1- <i>b</i>]chrysene	946
3.466	Dibenzo[<i>f,j</i>]picene	948
3.467	Dibenzo[<i>c,h</i>]pentaphene	950
3.468	Dibenzo[<i>a,o</i>]picene	952

3.469	Tribenzo[<i>a,c,j</i>]naphthacene	954
3.470	Dibenzo[<i>a,c</i>]pentaphene	956
3.471	Dibenzo[<i>b,f</i>]picene	958
3.472	Dibenzo[<i>a,c</i>]pentacene	960
3.473	Benzo[<i>a</i>]naphtho[1,2- <i>c</i>]naphthacene	962
3.474	Benzo[<i>p</i>]naphtho[2,1- <i>b</i>]chrysene	964
3.475	Benzo[<i>p</i>]naphtho[1,2- <i>b</i>]chrysene	966
3.476	Benzo[<i>a</i>]hexaphene	968
3.477	Phenanthro[1,2- <i>a</i>]naphthacene	970
3.478	Phenanthro[9,10- <i>b</i>]chrysene	972
3.479	Tribenzo[<i>b,g,k</i>]chrysene	974
3.480	Dinaphth[1,2- <i>a</i> :1',2'- <i>h</i>]anthracene	976
3.481	Benzo[<i>q</i>]hexaphene	978
3.482	Benzo[<i>c</i>]naphtho[2,3- <i>l</i>]chrysene	980
3.483	Benzo[<i>b</i>]naphtho[2,3- <i>l</i>]chrysene	982
3.484	Dibenzo[<i>b,j</i>]picene	984
3.485	Naphtho[1,2- <i>a</i>]pentacene	986
3.486	Dibenzo[<i>b,s</i>]picene	988
3.487	Naphtho[2,1- <i>a</i>]pentaphene	990
3.488	Phenanthro[9,10- <i>a</i>]naphthacene	992
3.489	Dibenzo[<i>a,c</i>]picene	994
3.490	Dibenzo[<i>c,s</i>]picene	996
3.491	Dibenzo[<i>a,m</i>]pentaphene	998
3.492	Naphtho[1,2- <i>b</i>]picene	1000
3.493	Benzo[<i>a</i>]naphtho[1,2- <i>j</i>]naphthacene	1002
3.494	Phenanthro[4,3- <i>b</i>]chrysene	1004
3.495	Dibenzo[<i>a,n</i>]picene	1006
3.496	Naphtho[2,1- <i>a</i>]picene	1008
3.497	Naphtho[2,1- <i>c</i>]pentaphene	1010
3.498	Naphtho[2,1- <i>c</i>]picene	1012
3.499	Benzo[<i>l</i>]naphtho[1,2- <i>b</i>]chrysene	1014
3.500	Benzo[<i>c</i>]naphtho[1,2- <i>l</i>]chrysene	1016
3.501	Benzo[<i>l</i>]naphtho[2,1- <i>b</i>]chrysene	1018
3.502	Heptaphene	1020
3.503	Benzo[<i>p</i>]hexaphene	1022
3.504	Benzo[<i>b</i>]naphtho[1,2- <i>l</i>]chrysene	1024
3.505	Benzo[<i>a</i>]naphtho[1,2- <i>l</i>]naphthacene	1026
3.506	Dibenzo[<i>a,n</i>]pentacene	1028
3.507	Benzo[<i>b</i>]naphtho[2,1- <i>k</i>]chrysene	1030
3.508	Phenanthro[2,1- <i>b</i>]chrysene	1032
3.509	Phenanthro[3,4- <i>a</i>]naphthacene	1034
3.510	Benzo[<i>o</i>]hexaphene	1036
3.511	Benzo[<i>c</i>]hexaphene	1038
3.512	Naphtho[2,3- <i>b</i>]picene	1040
3.513	Dibenzo[<i>b,n</i>]picene	1042

3.514	Dibenzo[<i>a,l</i>]pentacene1044
3.515	Naphtho[2,3- <i>c</i>]pentaphene1046
3.516	Dibenzo[<i>c,m</i>]pentaphene1048
3.517	Naphtho[1,2- <i>c</i>]pentaphene1050
3.518	Benzo[<i>a</i>]hexacene1052
3.519	Benzo[<i>a</i>]naphtho[2,1- <i>j</i>]naphthacene1054
3.520	Naphtho[2,1- <i>b</i>]picene1056
3.521	Dibenzo[<i>b,m</i>]picene1058
3.522	Anthra[2,1- <i>a</i>]naphthacene1060
3.523	Benzo[<i>b</i>]naphtho[1,2- <i>k</i>]chrysene1062
3.524	Phenanthro[1,2- <i>b</i>]chrysene1064
3.525	Dibenzo[<i>c,m</i>]picene1066
3.526	Heptacene1068
3.527	Ovalene1070
3.528	Dibenzo[<i>a,ghi</i>]naphtho[2,1,8- <i>cde</i>]perylene1072
3.529	Dibenzo[<i>a,cd</i>]naphtho[8,1,2,3- <i>fghi</i>]perylene1074
3.530	Benzo[<i>e</i>]phenanthro[2,3,4,5- <i>pqrab</i>]perylene1076
3.531	Dinaphtho[1,8- <i>ab:8',1',2',3'-fghi</i>]perylene1078
3.532	Dibenzo[<i>a,ghi</i>]naphtho[2,1,8- <i>lmn</i>]perylene1080
3.533	Dibenzo[<i>a,d</i>]coronene1082
3.534	Benzo[<i>h</i>]phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene1084
3.535	Dinaphtho[2,1,8- <i>fgh:7',8',1',2',3'-pqrst</i>]pentaphene1086
3.536	Pyreno[5,4,3,2,1- <i>pqrst</i>]pentaphene1088
3.537	Dinaphtho[2,1,8- <i>fgh:3',2',1',8',7'-rstuv</i>]pentaphene1090
3.538	Benzo[<i>e</i>]phenanthro[1,10,9,8- <i>opqra</i>]perylene1092
3.539	Benzo[3,4]phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene1094
3.540	Anthra[3,2,1,9- <i>pqra</i>]benzo[<i>cd</i>]perylene1096
3.541	Dibenzo[<i>a,ghi</i>]naphtho[8,1,2- <i>klm</i>]perylene1098
3.542	Dibenzo[<i>ghi,lm</i>]naphtho[1,8- <i>ab</i>]perylene1100
3.543	Dibenzo[<i>cd,k</i>]naphtho[3,2,1,8- <i>pqra</i>]perylene1102
3.544	Naphtho[1,2- <i>a</i>]coronene1104
3.545	Dibenzo[<i>fg,ij</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene1106
3.546	Anthra[2,1,9,8- <i>defgh</i>]benzo[<i>rst</i>]pentaphene1108
3.547	Dibenzo[<i>cd,n</i>]naphtho[3,2,1,8- <i>pqra</i>]perylene1110
3.548	Dibenzo[<i>a,g</i>]coronene1112
3.549	Dibenzo[<i>ghi,n</i>]naphtho[8,1,2- <i>bcd</i>]perylene1114
3.550	Benzo[<i>lm</i>]phenanthro[5,4,3- <i>abcd</i>]perylene1116
3.551	Dibenzo[<i>de,ij</i>]naphtho[7,8,1,2,3- <i>pqrst</i>]pentaphene1118
3.552	Anthra[3,2,1,9,8- <i>rstuva</i>]benzo[<i>ij</i>]pentaphene1120
3.553	Dibenzo[<i>de,ij</i>]naphtho[3,2,1,8,7- <i>rstuv</i>]pentaphene1122
3.554	Naphtho[2,3- <i>a</i>]coronene1124
3.555	Anthra[2,1,9,8,7- <i>defghi</i>]benzo[<i>st</i>]pentacene1126
3.556	Dibenzo[<i>a,j</i>]coronene1128
3.557	Anthra[2,1,9,8,7- <i>defghi</i>]benzo[<i>uv</i>]pentacene1130
3.558	Dinaphtho[2,1,8,7- <i>defg:2',1',8',7'-qrst</i>]pentacene1132

3.559	Dibenzo[<i>ij,rst</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene1134
3.560	Dinaphtho[2,1,8,7- <i>defg</i> :2',1',8',7'- <i>ijkl</i>]pentaphene1136
3.561	Dibenzo[<i>kl,rst</i>]naphtho[2,1,8,7- <i>defg</i>]pentaphene1138
3.562	Anthra[2,1,9,8,7- <i>defghi</i>]benzo[<i>op</i>]pentacene1140
3.563	Dinaphtho[2,1,8,7- <i>defg</i> :2',1',8',7'- <i>opqr</i>]pentacene1142
3.564	Anthra[7,8,9,1,2,3- <i>rstuvw</i>]hexaphene1144
3.565	Benzo[<i>def</i>]pyranthrene1146
3.566	Phenanthro[2,1,10,9,8,7- <i>tuvwxyz</i>]hexaphene1148
3.567	Dinaphtho[8,1,2- <i>cde</i> :7',8',1',2',3'- <i>pqrst</i>]pentaphene1150
3.568	Fluorantheno[8,9- <i>b</i>]triphenylene1152
3.569	Benzo[<i>h</i>]naphtho[1,2,3,4- <i>rst</i>]pentaphene1154
3.570	Tribenzo[<i>a,f,j</i>]perylene1156
3.571	Tetrabenzo[<i>a,c,hi,mn</i>]naphthacene1158
3.572	Anthra[1,2,3,4- <i>rst</i>]pentaphene1160
3.573	Dibenzo[<i>q,vwx</i>]hexaphene1162
3.574	Dibenzo[<i>fg,st</i>]hexacene1164
3.575	Naphtho[2,1,8- <i>yz</i> <i>a</i>]hexacene1166
3.576	Benzo[<i>tuv</i>]naphtho[2,1- <i>b</i>]picene1168
3.577	Benzo[<i>p</i>]naphtho[8,1,2- <i>abc</i>]coronene1170
3.578	Tribenzo[<i>a,ef,no</i>]coronene1172
3.579	Benzo[<i>bc</i>]naphtho[3,2,1- <i>ef</i>]coronene1174
3.580	Tribenzo[<i>a,ef,hi</i>]coronene1176
3.581	Benzo[<i>g</i>]naphtho[8,1,2- <i>abc</i>]coronene1178
3.582	Benzo[<i>bc</i>]naphtho[1,2,3- <i>ef</i>]coronene1180
3.583	Tribenzo[<i>a,hi,kl</i>]coronene1182
3.584	Anthra[9,1,2- <i>abc</i>]coronene1184
3.585	Dibenzo[<i>fg,ij</i>]phenanthro[2,1,10,9,8,7- <i>pqrstuv</i>]pentaphene1186
3.586	Perylo[3,2,1,12- <i>pqrab</i>]perylene1188
3.587	Benzo[<i>m</i>]naphtho[8,1,2- <i>abc</i>]coronene1190
3.588	Phenanthro[10,1,2- <i>abc</i>]coronene1192
3.589	Benzo[<i>j</i>]naphtho[8,1,2- <i>abc</i>]coronene1194
3.590	Benzo[<i>pqr</i>]dinaphtho[8,1,2- <i>bcd</i> :2',1',8'- <i>lmn</i>]perylene1196
3.591	Naphtho[3,2,1,8,7- <i>defgh</i>]pyranthrene1198
3.592	peri-Pentacenopentacene1200
3.593	Benzo[<i>a</i>]pyranthrene1202
3.594	Tetrabenzo[<i>a,cd,f,lm</i>]perylene1204
3.595	Dibenzo[<i>fgh,pqr</i>]trinaphthylene1206
3.596	Tetrabenzo[<i>a,cd,j,lm</i>]perylene1208
3.597	Dibenzo[<i>fg,ij</i>]naphtho[2,1,8- <i>uva</i>]pentaphene1210
3.598	Dibenzo[<i>j,lm</i>]naphtho[1,8- <i>ab</i>]perylene1212
3.599	Tetrabenzo[<i>de,h,kl,rst</i>]pentaphene1214
3.600	Tetrabenzo[<i>de,jk,op,uv</i>]pentacene1216
3.601	Tetrabenzo[<i>de,hi,op,st</i>]pentacene1218
3.602	Dibenzo[<i>a,rst</i>]naphtho[8,1,2- <i>cde</i>]pentaphene1220
3.603	Benzo[<i>rst</i>]phenanthro[1,10,9- <i>cde</i>]pentaphene1222

3.604	Benzo[<i>rst</i>]phenanthro[10,1,2- <i>cde</i>]pentaphene1224
3.605	Anthra[9,1,2- <i>cde</i>]benzo[<i>rst</i>]pentaphene1226
3.606	Dinaphtho[2,1,8- <i>jkl</i> :2',1',8'- <i>uva</i>]pentacene1228
3.607	Naphtho[2,1- <i>c</i> :7,8- <i>c'</i>]diphenanthrene1230
3.608	Phenanthro[2,1- <i>f</i>]picene1232
3.609	Benzo[<i>j</i>]benzo[2,1- <i>a</i> :3,4- <i>a'</i>]dianthracene1234
3.610	Tetrabenzo[<i>a,c,j,l</i>]naphthacene1236
3.611	Benzo[6,7]phenanthro[4,3- <i>b</i>]chrysene1238
3.612	Dinaphtho[2,1- <i>a</i> :1',2'- <i>l</i>]naphthacene1240
3.613	Benzo[<i>c</i>]naphtho[2,1- <i>m</i>]pentaphene1242
3.614	Dinaphtho[2,1- <i>a</i> :2',1'- <i>j</i>]naphthacene1244
3.615	Benzo[<i>a</i>]heptacene1246
3.616	Dinaphtho[1,2- <i>b</i> :1',2'- <i>k</i>]chrysene1248
3.617	Octacene1250
3.618	Dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>nop</i>]coronene1252
3.619	Dibenzo[<i>ef,no</i>]naphtho[8,1,2- <i>abc</i>]coronene1254
3.620	Anthra[1,9,8- <i>abcd</i>]benzo[<i>hi</i>]coronene1256
3.621	Tetrabenzo[<i>bc,ef,kl,no</i>]coronene1258
3.622	Benzo[<i>ef</i>]phenaleno[9,1,2- <i>abc</i>]coronene1260
3.623	Tetrabenzo[<i>bc,ef,hi,kl</i>]coronene1262
3.624	Dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>efg</i>]coronene1264
3.625	Dibenzo[<i>ef,hi</i>]naphtho[8,1,2- <i>abc</i>]coronene1266
3.626	Dibenzo[<i>kl,no</i>]naphtho[8,1,2- <i>abc</i>]coronene1268
3.627	Benz[<i>a</i>]ovalene1270
3.628	Dinaphtho[8,1,2- <i>abc</i> :8',1',2'- <i>ghi</i>]coronene1272
3.629	Dibenzo[<i>hi,kl</i>]naphtho[8,1,2- <i>abc</i>]coronene1274
3.630	Benz[4,10]anthra[1,9,8- <i>abcd</i>]coronene1276
3.631	Pyreno[1,10,9- <i>abc</i>]coronene1278
3.632	Dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>klm</i>]coronene1280
3.633	Pyreno[10,1,2- <i>abc</i>]coronene1282
3.634	Benz[<i>d</i>]ovalene1284
3.635	Dinaphtho[8,1,2- <i>abc</i> :2',1',8'- <i>hij</i>]coronene1286
3.636	Dinaphtho[8,1,2- <i>abc</i> :8',1',2'- <i>jkl</i>]coronene1288
3.637	Benzo[<i>qrs</i>]naphtho[3,2,1,8,7- <i>defgh</i>]pyranthrene1290
3.638	Decacyclene1292
3.639	Dibenzo[<i>fg,ij</i>]phenanthro[9,10,1,2,3- <i>pqrst</i>]pentaphene1295
3.640	Tribenzo[<i>fgh,pqr,za1b1</i>]trinaphthylene1297
3.641	Dibenzo[<i>j,lm</i>]phenanthro[5,4,3- <i>abcd</i>]perylene1299
3.642	Tribenzo[<i>jk,qr,uv</i>]naphtho[2,1,8,7- <i>defg</i>]pentacene1301
3.643	Dibenzo[<i>rs,vwx</i>]naphtho[2,1,8,7- <i>klmn</i>]hexaphene1303
3.644	Benzo[<i>rst</i>]pyreno[1,10,9- <i>cde</i>]pentaphene1305
3.645	Anthra[2,3- <i>a</i>]coronene1307
3.646	Dibenzo[<i>ij,rst</i>]phenanthro[9,10,1,2- <i>defg</i>]pentaphene1309
3.647	Benzo[<i>rst</i>]dinaphtho[8,1,2- <i>cde</i> :2',1',8'- <i>klm</i>]pentaphene1311
3.648	Tetrabenzo[<i>a,f,k,n</i>]perylene1313

3.649	Tetrabenzo[<i>a,e,j,o</i>]perylene1315
3.650	Dinaphtho[3,2,1- <i>fg:3',2',1'-qr</i>]pentacene1317
3.651	Tetrabenzo[<i>a,f,j,o</i>]perylene1319
3.652	Dibenzo[<i>f,j</i>]naphtho[1,2,3,4- <i>pqr</i>]picene1321
3.653	Dinaphtho[1,2,3- <i>fg:3',2',1'-qr</i>]pentacene1323
3.654	Dinaphtho[1,2- <i>b,2',1'-n</i>]perylene1325
3.655	Dinaphtho[3,2,1- <i>fg:1',2',3'-ij</i>]pentaphene1327
3.656	Dinaphtho[1,2,3- <i>fg:1',2',3'-qr</i>]pentacene1329
3.657	Tetrabenzo[<i>a,c,hi,qr</i>]pentacene1331
3.658	Dinaphtho[1,8- <i>bc:1',8'-mn</i>]picene1333
3.659	Pyreno[2,1- <i>b</i>]picene1335
3.660	Dibenzo[<i>b,tuv</i>]naphtho[2,1- <i>m</i>]picene1337
3.661	Diphenanthro[3,4- <i>c:4',3'-g</i>]phenanthrene1339
3.662	Tetrabenzo[<i>a,c,l,n</i>]pentacene1341
3.663	Dinaphtho[2,3- <i>c:2',3'-m</i>]pentaphene1343
3.664	Chryseno[2,1- <i>b</i>]picene1345
3.665	Nonacene1347

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1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) are molecules that exist on earth due to natural and man-made causes. They are a significant health concern as many PAH compounds are known to be carcinogenic. PAHs are generally thermodynamically stable and hydrophobic and thus have a tendency to accumulate in the environment and are difficult to remove. An understanding of various chemical properties of PAHs is an important part of gauging their impact on human health.

The motivation for this special publication comes from the present authors' interest in the chemistry of PAHs and the seminal work of Sander and Wise, previously published as *NIST Special Publication 922: Polycyclic Aromatic Hydrocarbon Structure Index (SP922)*.¹ This special publication cataloged 660 PAH structures and gave dimensional parameters that could be used to predict chromatographic retention times.² One of the motivations for the present work is the relative ease with which estimates of thermochemical properties can be derived from quantum chemical calculations. The present authors have recently completed a study of several quantum chemistry methods for producing high-quality enthalpies of formation at 298 K for a large number of PAH compounds and substituted PAH compounds.³ In this work, two methods for predicting enthalpies of formation at 298 K via a model chemistry (G3//B3LYP and G3(MP2)//B3LYP) were compared to results from B3LYP calculations extrapolated to a large basis set limit and to available experimental values. In all cases it was found that the calculated values of the enthalpies of formation compared favorably to experiment once a systematic correction was applied. This systematic correction was based on the composition of the PAH molecule and made use of a group additivity model. Full details are available elsewhere.³ The thermodynamic tables presented herein are an expansion of

the present authors' work on predicting enthalpies of formation of PAHs at 298 K. This special publication presents a number of thermodynamic quantities (described below) over a range of temperatures.

In the course of the work on PAH enthalpies of formation, the opportunity arose to disseminate the results through a variety of media. One of these is the present special publication. Another is a website that is available at <http://pah.nist.gov/>. The PAH website contains all of the information presented in this special publication as well as additional information not appropriate for this special publication or information whose presentation is well suited for presentation on a computer screen. An example of the former is the inclusion of predicted UV-Visible spectra on the website. An example of the latter is the presentation of three-dimensional structures for the PAH molecules via a web-based application that allows the structures to be visualized and manipulated by the user. It is intended that the website will grow to include more PAH molecules and to include more properties. The selection of new PAH molecules and new properties is intended to be driven by the end users. Those interested in expanding the web-based database are encouraged to contact the authors of the present publication.

The present special publication largely reproduces and extends the content of the previous special publication (SP922). This special publication contains 5 IUPAC Parent Compounds PAHs that were not part of SP922, bringing the total number of molecules in the present publication to 665. The length/width/breadth parameters (as described in SP922) have been updated based on molecular structures optimized at the B3LYP/cc-pVDZ level of theory. These new parameters change very little from the previously-published values found in SP922. The present special publication adds a few additional compound names, gives CAS number for compounds that were previously unavailable, and corrects a very few errors in SP922.

2. Calculations

2.1. Quantum Chemistry Calculations

All of the structural and thermodynamic property information presented in this special publication have been derived from quantum chemistry calculations carried out at the B3LYP/cc-pVDZ level of theory using the Gaussian 09 computational chemistry program.⁴ B3LYP is a density functional theory (DFT) method. In particular, B3LYP is a hybrid functional consisting of Becke's three-parameter exchange functional⁵ and the Lee-Yang-Parr⁶ correlation functional. The B3LYP method has been extensively tested and is routinely used in quantum chemistry calculations. DFT methods are known to produce reliable optimized geometries and give good results for a variety of chemical properties for many molecules. Nevertheless, accurate estimation of enthalpies of formation is a challenging task, and the B3LYP/cc-pVDZ results by themselves cannot produce reliable results. Thus, additional corrections have been applied to the results of these calculations to produce high-quality results. A full account of the methodologies used to produce enthalpies of formation at 298 K is given in another publication by the present authors, and the interested reader is directed to this publication for additional details.³ Some aspects of the computation of enthalpies of formation will be discussed briefly in the following subsections.

For the results presented in this special publication, an optimization of the nuclear geometry is carried out at the B3LYP/cc-pVDZ level of theory. The moment(s) of inertia (I_{α}) are calculated using this geometry. The nuclear hessian (i.e., the matrix of second derivatives of the total energy with respect to the nuclear coordinates) is evaluated at the optimized geometry. Vibrational frequencies

(ν) are derived by diagonalizing the mass-weighted matrix of second derivatives (force constants). For a molecular geometry that is a minimum on the potential energy surface (which corresponds to an equilibrium geometry appropriate for evaluating thermochemical properties), all $3N - 6$ (where N is the number of atoms) vibrational frequencies are positive and real-valued.

2.2. Enthalpies of Formation

Calculation of the enthalpy of formation from quantities produced as part of a quantum chemistry calculation is straightforward and is described in detail elsewhere.^{7,8} A brief summary is given here.

The enthalpy of formation ($\Delta_f H^\circ(T)$) as a function of temperature (T) may be derived as the difference between a thermodynamic term ($H_0(T)$) and the atomization energy of the molecules

$$\Delta_f H^\circ(T) = H_0(T) - E_{\text{atom}} \quad (2.1)$$

The thermodynamic term ($H_0(T)$) is computed as a sum of the differences between the atomic enthalpies of formation ($\Delta_f H_{\text{atom},i}^\circ(T)$) and the atomic enthalpy increments ($H_{\text{inc,atom},i}^\circ(T)$), the molecular enthalpy increment ($H_{\text{inc,molecule}}^\circ(T)$), and the molecular zero-point energy (E_{ZPE})

$$H_0(T) = \sum_{i=1}^N \left[\Delta_f H_{\text{atom},i}^\circ(T) - H_{\text{inc,atom},i}^\circ(T) \right] + H_{\text{inc,molecule}}^\circ + E_{\text{ZPE}} \quad (2.2)$$

where N is the number of atoms in the molecule. The two terms in the summation in the equation are experimental values taken from the CODATA tables⁹ where

$$H_{\text{inc,atom}}^\circ(T) = H_{\text{atom}}^\circ(T) - H_{\text{atom}}^\circ(0 \text{ K}) \quad (2.3)$$

The values of the remaining two terms are taken from the DFT calculations. The molecular enthalpy increment ($H_{\text{inc,molecule}}^\circ(T)$) is expressed as the difference between the enthalpy at temperature T and

the enthalpy at 0 K

$$H_{\text{inc,molecule}}^{\circ}(T) = H_{\text{molecule}}^{\circ}(T) - H_{\text{molecule}}^{\circ}(0 \text{ K}) \quad (2.4)$$

The calculation of the molecular enthalpy will be discussed in the following section. The ZPE is calculated from the vibrational frequencies as

$$E_{\text{ZPE}} = \frac{1}{2} \sum_{i=1}^{3N-6} \nu_i \quad (2.5)$$

The atomization energy is evaluated as the difference between the sum of the energies of the individual atoms (E_i) and the total energy of the molecule (E_{tot})

$$E_{\text{atom}} = \sum_{i=1}^N E_i - E_{\text{tot}} \quad (2.6)$$

Values for the atomic energies of the atoms (E_i) and for the total energy of the molecule (E_{tot}) are computed using quantum chemistry.

2.3. Empirical Corrections to Calculations

As mentioned above, the B3LYP/cc-pVDZ calculations by themselves are not sufficiently accurate to produce reliable estimates of the enthalpies of formation. The strategy that has been adopted is to apply corrections to the quantum chemistry results. There are two such corrections: an extrapolation of the total energy and a correction based on a group additivity scheme. Thus, the corrected enthalpy of formation may be written

$$\Delta_f H_{\text{corr}}^{\circ} = \Delta_f H_{\text{calc}}^{\circ} + \epsilon_{\text{corr}} \quad (2.7)$$

where it is understood that $\Delta_f H_{\text{calc}}^{\circ}$ is calculated using the extrapolated B3LYP total energy and ϵ_{corr} is a correction based on a group additivity scheme. The corrections are described below.

2.3.1. Extrapolation of the Total Energy

One of the significant shortcomings identified in the B3LYP/cc-pVDZ calculations was the use of a relatively small basis set (cc-pVDZ). The choice of basis set was largely determined by the desire to permit determination of accurate optimized geometries and calculation of the vibrational frequencies at a modest computational cost, even for larger molecules. The cc-pVDZ basis set achieves these goals quite well, at the expense of some of the total energy. In order to recover some of the total energy, a basis set extrapolation scheme due to Truhlar is employed.¹⁰ In this method, it is recognized that the total energy can be partitioned and each part can be extrapolated to a large basis set limit. In the present case, the B3LYP total energy (E_{tot}) is partitioned into contributions from the exchange functional (B3) and the correlation functional(LYP)

$$E_{\text{tot}}^{\text{B3LYP}} = E^{\text{B3}} + E^{\text{LYP}} \quad (2.8)$$

where it is understood that the term E^{B3} contains all parts of the total energy except the correlation energy, i.e., the nuclear-nuclear repulsion and kinetic energy terms are combined into the exchange energy term. Assuming that each of these terms approaches its large basis set limit value (E_{∞}) via a power law functional dependence, the extrapolated energy may be written

$$E_X^{\lambda} = E_{\infty}^{\lambda} + A^{\lambda} X^{-\alpha} \quad (2.9)$$

where λ represents either the B3 or LYP terms, X is an integer related to the basis set (e.g., $X = 2$ for the cc-pVDZ basis, $X = 3$ for the cc-pVTZ basis set), and α is a parameter that may be adjusted to produce an optimal fit to the data.

To use the extrapolation scheme described above, single point energy calculations were carried out at the B3LYP/cc-pVTZ ($X = 3$) level of theory at the B3LYP/cc-pVDZ ($X = 2$) optimized

geometry. The extrapolated B3LYP total energy is then written

$$E_{\text{extrap}}^{\text{B3LYP}} = \frac{3^\alpha E_3^{\text{B3}} - 2^\alpha E_2^{\text{B3}}}{3^\alpha - 2^\alpha} + \frac{3^\beta E_3^{\text{LYP}} - 2^\beta E_2^{\text{LYP}}}{3^\beta - 2^\beta} \quad (2.10)$$

where the superscripts B3 and LYP represent the contributions from the B3 exchange and LYP correlation functionals, the subscripts 2 and 3 represent the cc-pVDZ and cc-pVTZ basis sets, respectively, and α and β are adjustable parameters.

In order to optimize the value of the parameters α and β , single point energy calculations at the B3LYP/cc-pV6Z level of theory at the optimized B3LYP/cc-pVDZ geometry were carried out for 16 small PAHs. These values were used to obtain optimize parameters for the extrapolation to the large basis set limit using a Levenberg-Marquardt optimization algorithm.^{11,12}

2.3.2. Corrections Based on Group Additivity

The group additivity scheme employed in the present work uses atom-centered groups and is based on the work of Benson and coworkers.^{13,14} In order to describe the PAH molecules in this special publication in terms of atom-centered groups, nine unique groups are required. These are denoted CH2, CH2d, CCH, CdH, CdC, CbH, Cb, Cf, and Cp, and their descriptions are given in Table 2.1. In order to clearly illustrate these groups, their labels are superimposed on several molecules, shown in Figure 2.1.

The correction to the enthalpy of formation is written as a sum of the product of counts of base groups (denoted by their base group names) and a corresponding coefficient ($f(x)$, where x is a base group name)

$$\begin{aligned} \epsilon_{\text{corr}} = & n_{\text{CH2}}f(\text{CH2}) + n_{\text{CH2d}}f(\text{CH2d}) + n_{\text{CCH}}f(\text{CCH}) + n_{\text{CdH}}f(\text{CdH}) + n_{\text{CdC}}f(\text{CdC}) \\ & + (n_{\text{CbH}} - 6)f(\text{CbH}) + n_{\text{Cb}}f(\text{Cb}) + n_{\text{Cf}}f(\text{Cf}) + n_{\text{Cp}}f(\text{Cp}) \quad (2.11) \end{aligned}$$

It was found during parameter optimization that subtracting 6 from the number of CbH groups

CH2	sp^3 methylene group, $-\text{CH}_2-$
CH2d	sp^3 methylene group adjacent to sp^2 group, $-\text{CH}_2-\text{C}=\text{C}$
CCH	sp^3 methylidyne group, $-\text{CH}<$
CdH	sp^2 alkene group bonded to a single sp^3 group, $-\text{CH}=\text{C}$
CdC	sp^2 isoalkene group bonded to two sp^3 groups, $>\text{C}=\text{C}$
CbH	aromatic carbon terminated by hydrogen
Cb	aromatic carbon terminated by carbon
Cf	fused aromatic carbon connected to one Cf or Cp group
Cp	pericondensed aromatic carbon (interior) connected to two Cf or Cp groups
CH3	terminal methyl group, $-\text{CH}_3$
CCC	methanetetrayl group, $>\text{C}<$
CdH2	terminal methylene group, $=\text{CH}_2$
CtH	terminal triple-bonded terminal carbon, $\equiv\text{CH}$
Ct	triple-bonded carbon, $\equiv\text{C}-$

Table 2.1: Base group names and descriptions used in group-based error correction scheme used in the B3LYP-based scheme.

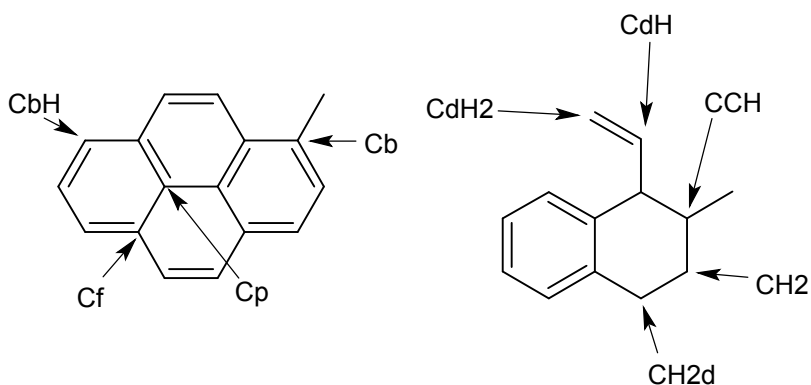


Figure 2.1: Atom-centered groups needed for describing PAH molecules included in this special publication. 1-methylpyrene and 2-methyl-1-vinyl-1,2,3,4-tetrahydronaphthalene are depicted with group identifiers indicated.

(as reflected in the equation above) significantly improved the overall results (in the sense that the fitting error was reduced). However, this has the drawback that no correction is applied to benzene.

Fitting was performed by minimizing the least squares difference between calculated and experimental values of the enthalpy of formation. Due to the relatively small number of PAHs for which an experimental determination of the enthalpy of formation was available, hydrocarbon-substituted PAHs with experimental enthalpies of formation were added to the fitting set. An additional five base groups (CH₃, CCC, CdH₂, CtH, Ct) whose descriptions are given in Table 2.1 were included to represent the added molecules. After correction, it was found that the mean unsigned deviation and the root mean squared deviation of the calculated results from the experimental data were 5.0 kJ/mol and 6.4 kJ/mol, respectively.

2.3.3. Additional Corrections to the Enthalpy of Formation

All enthalpies of formation in the tables are based on our extrapolated and empirically corrected B3LYP calculations, except for a number of PAHs where reliable experimentally-derived enthalpies of formation are available. These values, reported uncertainties, and references are give in Table 2.2. In cases where an experimental determination of the enthalpy of formation is available, the computed value of the enthalpy of formation in the table is corrected to the experimental value such that the value of the enthalpy of formation is correct at 298.15 K and is linearly adjusted at all other temperatures based on the difference between the computed and experimental values at 298.15 K. This is summarized in the following equation

$$\Delta_f H^\circ(T) = \Delta_f H_{\text{calc}}^\circ(T) - [\Delta_f H_{\text{calc}}^\circ(298.15 \text{ K}) - \Delta_f H_{\text{expt}}^\circ(298.15 \text{ K})] \quad (2.12)$$

In addition to employing experimentally-derived enthalpies of formation, where available, we compared our computed entropies $S^\circ(300 \text{ K})$, heat capacities $C_p^\circ(300\text{K to } 1500 \text{ K})$, and enthalpies $H(1500 \text{ K}) - H(0 \text{ K})$ to available values in the literature for about 25 molecules. In general, the comparisons were in good agreement with the differences for entropies, heat capacities, and

enthalpies on the order of less than 2 J/mol/K, 2 J/mol/K, and 1.5 kJ/mol, respectively. For several molecules, however, there was substantial disagreement between our computed values and those found in the TRC Thermodynamics Tables¹⁵ and in the TRC Web Thermo Tables (WTT)¹⁶. The differences in entropies were as much as (20 to 40) J/mol/K in entropy at 300 K, with corresponding differences in heat capacities. The molecules with significant differences were biphenylene, benzo[c]phenanthrene, chrysene, triphenylene, perylene, azulene, and coronene. For chrysene, triphenylene, perylene, and coronene there were substantial differences between the printed TRC Tables and the online WTT versions which we determined were results of employing Wilhoit polynomials in the WTT to estimate the heat capacities. Those values in the printed TRC Tables were computed using statistical mechanics using estimated force constants from phenanthrene for the vibrational modes. They are in better agreement with our values – however, there are still differences on the order of (4 to 8) J/mol/K for entropies at 300 K. We believe our computed thermodynamic functions are correct since we are employing directly computed vibrational frequencies in the statistical mechanics calculations – rather than using estimation methods. An extended comparison of the JANAF table for C₂H₄ to our computed values (not included in this special publication) shows that the only significant errors are for the enthalpy of formation and for the entropy. The mean unsigned deviation in the enthalpy of formation using the correction scheme described above is 5 kJ/mol.³ The deviation in the entropy from the JANAF value at 298 K was approximately 7 J/mol K. This deviation increases the discrepancy between the JANAF Table values of the Gibbs free energy and Gibbs energy of formation versus the computed result as a function of increasing temperature (as might be expected). Correcting the value of the entropy at 298 K and applying this same correction over the entire temperature range led to values in excellent agreement with the values published in the JANAF Tables.

Formula	Name	$\Delta_f H^\circ(295.15 \text{ K})$	Uncertainty	Reference
C_6H_6	Benzene	82.9	0.9	[17]
C_9H_8	Indene	161.2	2.3	[17]
C_{10}H_8	Naphthalene	150.6	1.6	[17]
$\text{C}_{12}\text{H}_{10}$	Acenaphthene	156.8	3.1	[17]
C_{12}H_8	Acenaphthylene	263.2	3.7	[17]
C_{12}H_8	Biphenylene	417.2	1.9	[17]
$\text{C}_{13}\text{H}_{10}$	Fluorene	179.4	3.	[18]
$\text{C}_{14}\text{H}_{10}$	Anthracene	230.9	3.7	[17]
$\text{C}_{14}\text{H}_{10}$	Phenanthrene	201.4	3.5	[17]
$\text{C}_{16}\text{H}_{10}$	Fluoranthene	282.4	2.8	[19]
$\text{C}_{16}\text{H}_{10}$	Pyrene	225.5	4.3	[17]
$\text{C}_{18}\text{H}_{12}$	Benz[a]anthracene	290.3	6.	[17]
$\text{C}_{18}\text{H}_{12}$	Benzo[c]phenanthrene	295.3	9.1	[17]
$\text{C}_{18}\text{H}_{12}$	Chrysene	268.5	2.8	[17]
$\text{C}_{18}\text{H}_{12}$	Triphenylene	270.1	3.1	[17]
$\text{C}_{20}\text{H}_{12}$	Benzo[a]pyrene	296.9	5.5	[17]
$\text{C}_{20}\text{H}_{12}$	Perylene	319.4	2.2	[20]
$\text{C}_{24}\text{H}_{12}$	Coronene	294.9	11.1	[17]

Table 2.2: Experimental values and uncertainties (typically 2σ) of the enthalpy of formation ($\Delta_f H^\circ(298.15 \text{ K})$, kJ/mol) used to correct computed values in the tables. Please see the original reference for more information.

Quantity	Value	Description
m_{H}	1.00794 u	mass of hydrogen atom
m_{C}	12.0107 u	mass of carbon atom
R	8.314 472 J/mol K	molar gas constant
h	$6.626\,069\,57 \times 10^{-34}$ J s	Planck constant
k	$1.380\,6488 \times 10^{-23}$ J/K	Boltzmann constant

Table 2.3: Values of masses and constants used to compute table entries.

2.4. Thermodynamic Tables

The format of the data presented mimics the format of the NIST-JANAF tables^[21] as closely as possible. Thermodynamic properties of the PAH molecules were computed using the machinery of statistical mechanics via quantities derived from the DFT calculation. The quantities of interest are the heat capacity at constant pressure (C_p), the entropy (S) and an enthalpy-like derived term (described below), the enthalpy increment ($H^\circ(T) - H^\circ(T_r)$ where $T_r = 298.15$ K, the enthalpy of formation ($\Delta_f H^\circ$, defined above), the Gibbs energy of formation, and the logarithm of the equilibrium constant of formation.

A number of these quantities are computed as sums of electronic, vibrational, rotational, and translational terms as indicated below. The formulae given in the following sections may be found in many textbooks on Statistical Mechanics (e.g., the book by McQuarrie^[22]). The NIST-JANAF tables^[21] contain a useful summary of many of the formulae needed to compute the quantities of interest.

The values of the various masses and constants used in the calculations are provided in Table 2.3.

2.4.1. Heat Capacity at Constant Pressure

The heat capacity at constant pressure is expressed as a sum of vibrational, rotational, and translational contributions (the electronic contribution is zero)

$$C_p^\circ(T) = C_{p,\text{vib}}^\circ(T) + C_{p,\text{rot}}^\circ + C_{p,\text{trans}}^\circ \quad (2.13)$$

where

$$C_{p,\text{vib}}^\circ(T) = R\hbar^2\beta^2 \sum_{i=1}^{3N-6} \frac{v_i^2 e^{\hbar\beta v_i}}{(e^{\hbar\beta v_i} - 1)^2} \quad (2.14)$$

and R is the molar gas constant, $\hbar = h/2\pi$, h is Planck's constant, $\beta = 1/kT$, and k is Boltzmann's constant. The rotational contribution is

$$C_{p,\text{rot}}^\circ = \frac{3}{2}R \quad (2.15)$$

and the translational contribution is

$$C_{p,\text{trans}}^\circ = \frac{5}{2}R \quad (2.16)$$

2.4.2. Entropy

The entropy is defined as a sum of electronic, vibrational, rotational, and translational terms

$$S^\circ(T) = S_{\text{elec}}^\circ + S_{\text{vib}}^\circ(T) + S_{\text{rot}}^\circ(T) + S_{\text{trans}}^\circ(T) \quad (2.17)$$

where

$$S_{\text{elec}}^\circ = R \ln q_{\text{elec}} \quad (2.18)$$

$$S_{\text{vib}}^\circ(T) = R \sum_{i=1}^{3N-6} \left[\frac{\hbar\beta v_i}{e^{\hbar\beta v_i} - 1} - \ln(1 - e^{-\hbar\beta v_i}) \right] \quad (2.19)$$

$$S_{\text{rot}}^\circ(T) = R \left[\frac{3}{2} + \ln q_{\text{rot}}(T) \right] \quad (2.20)$$

$$S_{\text{trans}}^{\circ}(T) = R \frac{5}{2} + \ln q_{\text{trans}}(T) \quad (2.21)$$

where the electronic partition function (q_{elec}) is taken to be equal to the spin multiplicity of the molecule (in the absence of information about electronically excited states), the rotational partition function (q_{rot}) is

$$q_{\text{rot}}(T) = \frac{1}{\sigma} \pi \left(\frac{8\pi^2 kT}{h^2} \right) I_A I_B I_C^{1/2} \quad (2.22)$$

for a nonlinear polyatomic molecule, where σ is a symmetry number and I_A , I_B , and I_C are the principal moments of inertia. The translational partition function (q_{trans}) is

$$q_{\text{trans}}(T) = \left(\frac{MkT}{h} \right)^{3/2} kT \quad (2.23)$$

where M is the molecular mass. An additional entropy-like term is reported in the tables. It is computed as

$$- \frac{G^{\circ}(T) - H^{\circ}(T_r)}{T} \quad (2.24)$$

where $T_r = 298.15$ K.

2.4.3. Enthalpy

The molecular enthalpy is computed as a sum of vibrational, rotational, and translational terms

$$H^{\circ}(T) = H_{\text{vib}}^{\circ}(T) + H_{\text{rot}}^{\circ}(T) + H_{\text{trans}}^{\circ}(T) \quad (2.25)$$

where the vibrational contribution is defined

$$H_{\text{vib}}^{\circ}(T) = E_{\text{ZPE}} + RT \sum_{i=1}^{3N-6} \frac{\hbar\beta\nu_i}{e^{\hbar\beta\nu_i} - 1} \quad (2.26)$$

the rotation contribution is defined

$$H_{\text{rot}}^{\circ}(T) = \frac{3}{2}RT \quad (2.27)$$

and the translational contribution is defined

$$H_{\text{trans}}^{\circ}(T) = \frac{5}{2}RT \quad (2.28)$$

In the tables, the enthalpy is reported as an enthalpy increment ($H^{\circ}(T) - H^{\circ}(T_r)$) from a reference temperature ($T_r = 298.15$ K).

2.4.4. Gibbs Energy of Formation

The Gibbs energy of formation is computed from the enthalpy of formation and entropy of the molecule using

$$\Delta_f G^{\circ}(T) = \Delta_f H^{\circ}(T) - T\Delta S^{\circ} \quad (2.29)$$

2.4.5. Equilibrium Constant of Formation

The equilibrium constant of formation (K_f) is related to the Gibbs energy of formation via

$$\Delta_f G^{\circ}(T) = -RT \ln K_f \quad (2.30)$$

The entry given in the tables is the logarithm (i.e., common or base 10) of the equilibrium constant of formation, which is found from the relation

$$\log K_f = -\frac{\Delta_f G^{\circ}(T)}{2.3026 RT} \quad (2.31)$$

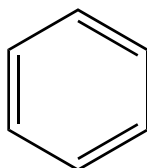
3. Tables

Tables of thermodynamic properties, the *raison d'être* for this special publication, are given for 665 polycyclic aromatic hydrocarbons on the following pages. The various properties that are tabulated and the means of their calculation have been described in the previous section. Presentation of the data is made in a 2-page format.

On the first of these two pages, several pieces of descriptive data are given including the name and any alternate names (if available) of the PAH, the chemical formula and molecular mass of the PAH, and the CAS registry number. A 2-dimensional structural depiction of the molecule is also given on this page. This structural representation is a “stick diagram” with implicit hydrogen atoms. The location of the hydrogen atoms is readily deduced from the structural drawing and the molecular formula. The last items on the first page are measurements of the length, width, and breadth of the molecule when confined to a minimal bounding box. These parameters are important in estimating chromatographic retention times and were included in the original Special Publication (SP922) of Sander and Wise.^[1] The parameters included in the present publication have been updated based on the optimized B3LYP geometries (see the full paper^[3] for more details).

The second data page consists entirely of a table of thermodynamic properties given as a function of temperature, with temperature ranging from 0 K to 5000 K. The format of this table has been designed to mimic the layout of a table in the NIST-JANAF Tables.^[21]

3.1. Benzene



Other names: [6] Annulene
Benzine
Benzol
Cyclohexatriene
Phene

Formula: C₆H₆
Mass: 78.112 g/mol
CAS Number: 71-43-2
Point Group: D_{6h}

Length: 7.372 Å
Width: 6.706 Å
Breadth: 3.884 Å
L/B Ratio: 1.099

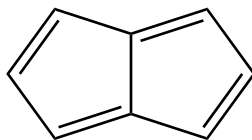
Cartesian coordinates:

C	-0.6224	-1.2440	0.0000	C	-0.7661	1.1611	0.0000	H	2.4814	0.1481	0.0000
C	0.7661	-1.1611	0.0000	C	-1.3886	-0.0829	0.0000	H	1.1125	2.2230	0.0000
C	1.3886	0.0830	0.0000	H	-1.1126	-2.2229	0.0000	H	-1.3694	2.0746	0.0000
C	0.6224	1.2440	0.0000	H	1.3692	-2.0747	0.0000	H	-2.4813	-0.1483	0.0000

Table 3.1: Table of thermodynamic data as a function of temperature for Benzene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			$\log K_f$
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-14.321	85.038	85.038	∞
100	35.309	213.922	323.537	-10.962	94.288	103.686	-54.159
200	53.599	243.018	276.321	-6.660	88.552	115.293	-30.111
250	67.921	256.476	271.003	-3.632	85.616	122.318	-25.556
298.15	83.019	269.722	269.722	0.000	82.900	129.637	-22.711
300	83.606	270.237	269.723	0.154	82.799	129.928	-22.622
350	99.272	284.308	270.799	4.728	80.200	137.992	-20.594
400	114.065	298.543	273.376	10.067	77.856	146.409	-19.119
450	127.590	312.772	276.964	16.114	75.752	155.106	-18.004
500	139.754	326.856	281.251	22.803	73.867	164.030	-17.136
600	160.344	354.227	291.150	37.846	70.655	182.377	-15.877
700	176.904	380.232	302.035	54.737	68.094	201.209	-15.014
800	190.467	404.768	313.359	73.127	66.099	220.365	-14.388
900	201.767	427.874	324.812	92.756	64.596	239.740	-13.914
1000	211.300	449.639	336.217	113.422	63.512	259.263	-13.542
1100	219.409	470.169	347.470	134.968	62.777	278.878	-13.243
1200	226.347	489.565	358.511	157.265	62.334	298.543	-12.995
1300	232.313	507.924	369.304	180.205	62.117	318.238	-12.787
1400	237.463	525.333	379.833	203.700	62.080	337.944	-12.609
1500	241.926	541.872	390.089	227.675	62.187	357.648	-12.454
1600	245.809	557.613	400.071	252.066	62.395	377.338	-12.319
1700	249.201	572.619	409.783	276.820	62.675	397.006	-12.198
1800	252.174	586.949	419.231	301.892	63.003	416.673	-12.091
1900	254.791	600.655	428.421	327.243	63.364	436.309	-11.995
2000	257.103	613.784	437.363	352.840	63.737	455.930	-11.907
2100	259.153	626.378	446.066	378.655	64.100	475.529	-11.828
2200	260.977	638.477	454.539	404.664	64.450	495.115	-11.755
2300	262.605	650.115	462.791	430.844	64.779	514.681	-11.689
2400	264.064	661.322	470.831	457.179	65.071	534.225	-11.627
2500	265.375	672.129	478.668	483.652	65.324	553.784	-11.570
2600	266.556	682.561	486.311	510.250	65.528	573.306	-11.518
2700	267.625	692.641	493.767	536.959	65.681	592.835	-11.469
2800	268.594	702.392	501.045	563.771	65.778	612.370	-11.424
2900	269.474	711.832	508.151	590.675	65.808	631.887	-11.381
3000	270.277	720.982	515.094	617.663	65.781	651.409	-11.342
3100	271.010	729.856	521.879	644.728	65.678	670.918	-11.305
3200	271.682	738.471	528.514	671.863	65.507	690.447	-11.270
3300	272.299	746.841	535.004	699.063	65.263	709.991	-11.238
3400	272.866	754.978	541.354	726.322	64.940	729.526	-11.208
3500	273.389	762.896	547.572	753.635	64.536	749.067	-11.179
3600	273.872	770.604	553.660	780.998	64.056	768.636	-11.152
3700	274.319	778.114	559.626	808.408	63.494	788.231	-11.128
3800	274.733	785.435	565.472	835.861	62.840	807.821	-11.104
3900	275.118	792.577	571.204	863.353	62.105	827.423	-11.082
4000	275.476	799.547	576.826	890.883	61.285	847.075	-11.061
4100	275.809	806.353	582.341	918.448	60.371	866.730	-11.042
4200	276.120	813.003	587.754	946.044	59.368	886.407	-11.024
4300	276.411	819.504	593.069	973.671	58.273	906.088	-11.007
4400	276.683	825.862	598.287	1001.326	57.089	925.818	-10.991
4500	276.938	832.082	603.414	1029.007	55.817	945.592	-10.976
4600	277.178	838.172	608.451	1056.713	54.447	965.391	-10.962
4700	277.403	844.135	613.403	1084.442	52.980	985.196	-10.949
4800	277.614	849.978	618.271	1112.193	51.430	1005.057	-10.937
4900	277.813	855.704	623.058	1139.965	49.778	1024.922	-10.926
5000	278.001	861.318	627.767	1167.755	48.045	1044.868	-10.915

3.2. Pentalene



Formula: C₈H₆
Mass: 102.133 g/mol
CAS Number: 250-25-9
Point Group: D_{2h}

Length: 8.883 Å
Width: 6.791 Å
Breadth: 3.882 Å
L/B Ratio: 1.308

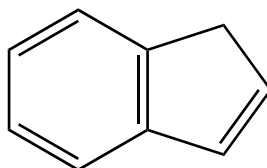
Cartesian coordinates:

C	-1.3859	1.1770	0.0000	C	2.1548	-0.0571	0.0000	H	-1.6938	-2.1719	0.0000
C	-2.1548	0.0571	0.0000	C	1.2981	1.1588	0.0000	H	1.6938	2.1719	0.0000
C	-1.2982	-1.1589	0.0000	C	0.0141	0.7466	0.0000	H	3.2414	-0.0053	0.0000
C	-0.0141	-0.7466	0.0000	H	-3.2414	0.0052	0.0000	H	1.7103	-2.2148	0.0000
C	1.3859	-1.1770	0.0000	H	-1.7099	2.2150	0.0000				

Table 3.2: Table of thermodynamic data as a function of temperature for Pentalene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-17.895	390.740	390.740	∞
100	42.769	237.197	379.818	-14.262	400.810	408.070	-213.149
200	70.242	274.136	318.024	-8.778	395.604	417.355	-109.000
250	89.673	291.862	311.013	-4.788	393.038	423.091	-88.398
298.15	109.172	309.325	309.325	0.000	390.740	429.092	-75.174
300	109.914	310.003	309.327	0.203	390.655	429.330	-74.751
350	129.359	328.423	310.738	6.190	388.528	435.949	-65.060
400	147.203	346.882	314.103	13.112	386.662	442.850	-57.829
450	163.177	365.160	318.763	20.879	385.023	449.974	-52.231
500	177.313	383.100	324.303	29.399	383.572	457.276	-47.770
600	200.808	417.593	337.005	48.353	381.116	472.257	-41.113
700	219.339	449.993	350.857	69.395	379.160	487.610	-36.385
800	234.289	480.291	365.164	92.102	377.640	503.208	-32.855
900	246.603	508.620	379.547	116.165	376.501	518.972	-30.120
1000	256.901	535.151	393.795	141.355	375.695	534.849	-27.937
1100	265.605	560.055	407.789	167.492	375.163	550.794	-26.155
1200	273.018	583.492	421.464	194.433	374.862	566.773	-24.670
1300	279.371	605.603	434.787	222.061	374.735	582.773	-23.416
1400	284.841	626.511	447.741	250.278	374.740	598.779	-22.340
1500	289.573	646.329	460.326	279.004	374.850	614.780	-21.408
1600	293.684	665.151	472.544	308.172	375.025	630.770	-20.592
1700	297.271	683.066	484.405	337.724	375.239	646.739	-19.871
1800	300.413	700.148	495.920	367.611	375.468	662.715	-19.231
1900	303.176	716.467	507.101	397.794	375.702	678.662	-18.657
2000	305.617	732.081	517.963	428.236	375.923	694.605	-18.141
2100	307.779	747.045	528.518	458.908	376.105	710.533	-17.673
2200	309.703	761.408	538.779	489.784	376.247	726.456	-17.248
2300	311.420	775.214	548.761	520.841	376.348	742.371	-16.859
2400	312.958	788.501	558.475	552.062	376.385	758.269	-16.503
2500	314.339	801.305	567.934	583.428	376.362	774.202	-16.176
2600	315.585	813.658	577.149	614.925	376.265	790.101	-15.873
2700	316.711	825.590	586.130	646.541	376.097	806.026	-15.593
2800	317.731	837.127	594.890	678.264	375.848	821.968	-15.334
2900	318.659	848.293	603.436	710.084	375.511	837.902	-15.092
3000	319.505	859.110	611.779	741.993	375.097	853.857	-14.867
3100	320.277	869.599	619.928	773.982	374.582	869.806	-14.656
3200	320.985	879.779	627.890	806.046	373.980	885.794	-14.459
3300	321.635	889.667	635.673	838.178	373.283	901.813	-14.274
3400	322.232	899.277	643.286	870.371	372.485	917.830	-14.100
3500	322.783	908.626	650.734	902.622	371.585	933.867	-13.937
3600	323.291	917.726	658.025	934.926	370.590	949.955	-13.783
3700	323.762	926.591	665.164	967.279	369.491	966.080	-13.638
3800	324.198	935.231	672.158	999.678	368.278	982.215	-13.501
3900	324.604	943.657	679.012	1032.118	366.966	998.371	-13.371
4000	324.980	951.880	685.731	1064.597	365.547	1014.602	-13.249
4100	325.332	959.909	692.321	1097.113	364.012	1030.847	-13.133
4200	325.659	967.753	698.786	1129.663	362.369	1047.129	-13.023
4300	325.966	975.420	705.130	1162.244	360.612	1063.423	-12.918
4400	326.252	982.917	711.359	1194.855	358.746	1079.789	-12.818
4500	326.521	990.251	717.475	1227.494	356.774	1096.216	-12.724
4600	326.773	997.431	723.483	1260.159	354.681	1112.688	-12.635
4700	327.010	1004.461	729.387	1292.848	352.470	1129.173	-12.549
4800	327.232	1011.348	735.190	1325.560	350.157	1145.738	-12.468
4900	327.442	1018.098	740.895	1358.294	347.719	1162.312	-12.390
5000	327.640	1024.715	746.505	1391.048	345.184	1178.995	-12.317

3.3. Indene



Other names: 1*H*-Indene
Formula: C₉H₈
Mass: 116.160 g/mol
CAS Number: 95-13-6
Point Group: C_s

Length: 9.156 Å
Width: 7.306 Å
Breadth: 4.173 Å
L/B Ratio: 1.253

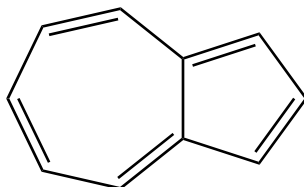
Cartesian coordinates:

C	2.1798	-0.6160	0.0000	C	-1.6562	1.1134	0.0000	H	1.0505	-2.4704	0.0000
C	2.1323	0.7751	0.0000	C	-2.4376	0.0122	0.0000	H	-1.9739	2.1546	0.0000
C	0.9130	1.4535	0.0000	C	-1.6048	-1.2432	0.0000	H	-3.5253	-0.0222	0.0000
C	1.0091	-1.3771	0.0000	H	3.1502	-1.1232	0.0000	H	-1.8103	-1.8673	0.8888
C	-0.2024	-0.7110	0.0000	H	3.0660	1.3470	0.0000	H	-1.8103	-1.8673	-0.8888
C	-0.2512	0.7025	0.0000	H	0.8753	2.5468	0.0000				

Table 3.3: Table of thermodynamic data as a function of temperature for Indene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-19.859	166.663	166.663	∞
100	45.849	254.805	416.526	-16.172	175.819	191.486	-100.020
200	80.009	296.116	346.208	-10.018	168.263	210.117	-54.876
250	102.302	316.323	338.202	-5.470	164.563	221.009	-46.176
298.15	124.940	336.273	336.273	0.000	161.200	232.192	-40.678
300	125.810	337.049	336.276	0.232	161.076	232.632	-40.504
350	148.860	358.188	337.892	7.103	157.912	244.814	-36.536
400	170.411	379.492	341.760	15.093	155.106	257.421	-33.615
450	190.005	400.715	347.134	24.112	152.629	270.361	-31.382
500	207.564	421.660	353.542	34.059	150.446	283.569	-29.624
600	237.163	462.223	368.303	56.352	146.821	310.550	-27.035
700	260.843	500.626	384.490	81.295	144.055	338.071	-25.227
800	280.127	536.757	401.289	108.375	142.034	365.929	-23.892
900	296.098	570.702	418.246	137.210	140.658	394.000	-22.867
1000	309.493	602.612	435.104	167.509	139.834	422.198	-22.053
1100	320.827	632.656	451.711	199.040	139.463	450.459	-21.390
1200	330.481	660.997	467.982	231.618	139.470	478.731	-20.838
1300	338.747	687.784	483.869	265.090	139.767	506.993	-20.371
1400	345.858	713.155	499.348	299.329	140.290	535.226	-19.969
1500	352.003	737.231	514.412	334.229	140.992	563.415	-19.619
1600	357.336	760.123	529.059	369.703	141.817	591.549	-19.312
1700	361.984	781.929	543.298	405.674	142.724	619.619	-19.038
1800	366.051	802.737	557.137	442.080	143.681	647.659	-18.794
1900	369.624	822.626	570.591	478.868	144.670	675.626	-18.574
2000	372.777	841.668	583.672	515.991	145.662	703.549	-18.374
2100	375.568	859.924	596.395	553.411	146.627	731.418	-18.193
2200	378.050	877.454	608.775	591.094	147.561	759.245	-18.026
2300	380.263	894.309	620.825	629.012	148.458	787.026	-17.874
2400	382.244	910.535	632.561	667.139	149.291	814.755	-17.732
2500	384.023	926.176	643.994	705.454	150.061	842.491	-17.603
2600	385.625	941.269	655.139	743.938	150.753	870.156	-17.481
2700	387.073	955.851	666.008	782.574	151.367	897.818	-17.369
2800	388.385	969.952	676.613	821.348	151.893	925.472	-17.265
2900	389.578	983.602	686.965	860.247	152.318	953.087	-17.167
3000	390.664	996.828	697.074	899.260	152.657	980.697	-17.075
3100	391.656	1009.654	706.952	938.377	152.882	1008.274	-16.989
3200	392.565	1022.103	716.607	977.588	153.005	1035.869	-16.908
3300	393.398	1034.196	726.048	1016.887	153.020	1063.474	-16.833
3400	394.165	1045.951	735.285	1056.266	152.918	1091.055	-16.762
3500	394.871	1057.388	744.325	1095.718	152.697	1118.632	-16.694
3600	395.523	1068.521	753.177	1135.238	152.365	1146.243	-16.631
3700	396.127	1079.366	761.847	1174.821	151.912	1173.878	-16.572
3800	396.686	1089.938	770.342	1214.462	151.325	1201.499	-16.515
3900	397.206	1100.248	778.670	1254.157	150.621	1229.125	-16.462
4000	397.689	1110.311	786.835	1293.902	149.792	1256.816	-16.412
4100	398.139	1120.137	794.845	1333.694	148.826	1284.503	-16.364
4200	398.558	1129.736	802.705	1373.529	147.732	1312.212	-16.319
4300	398.951	1139.119	810.420	1413.404	146.503	1339.918	-16.276
4400	399.318	1148.295	817.995	1453.318	145.146	1367.687	-16.236
4500	399.662	1157.272	825.435	1493.267	143.662	1395.511	-16.198
4600	399.984	1166.060	832.745	1533.250	142.036	1423.365	-16.162
4700	400.287	1174.665	839.929	1573.263	140.269	1451.219	-16.128
4800	400.573	1183.096	846.990	1613.306	138.382	1479.148	-16.096
4900	400.841	1191.358	853.934	1653.377	136.347	1507.072	-16.065
5000	401.094	1199.459	860.764	1693.474	134.197	1535.108	-16.037

3.4. Azulene



Other names: bicyclo[5.3.0]decapentaene

Formula: $C_{10}H_8$

Mass: 128.17 g/mol

CAS Number: 275-51-4

Point Group: C_{2v}

Length: 9.809 Å

Width: 7.738 Å

Breadth: 3.886 Å

L/B Ratio: 1.268

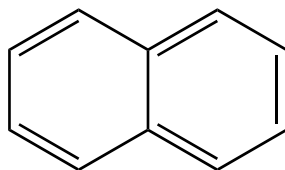
Cartesian coordinates:

C	-0.0241	1.3828	0.0094	C	1.1742	4.3383	0.0148	H	3.2822	0.6273	-0.0254
C	-0.0088	-0.0257	0.0011	C	-0.2129	4.5306	0.0283	H	2.9831	3.2329	-0.0080
C	1.3306	-0.4583	-0.0134	C	-1.2491	3.5886	0.0320	H	1.7786	5.2501	0.0143
C	2.1930	0.6542	-0.0153	C	-1.1606	2.1909	0.0234	H	-0.5367	5.5769	0.0380
C	1.4109	1.8261	-0.0013	H	-0.8931	-0.6622	0.0058	H	-2.2628	3.9998	0.0435
C	1.8913	3.1353	0.0015	H	1.6518	-1.5011	-0.0221	H	-2.1157	1.6532	0.0282

Table 3.4: Table of thermodynamic data as a function of temperature for Azulene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			$\log K_f$
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-21.719	280.872	280.872	∞
100	50.017	255.858	434.530	-17.867	294.787	310.444	-162.156
200	88.771	301.496	356.810	-11.063	287.555	328.950	-85.911
250	113.030	323.876	347.978	-6.026	284.049	339.705	-70.976
298.15	137.255	345.855	345.855	0.000	280.872	350.718	-61.443
300	138.180	346.707	345.858	0.255	280.755	351.151	-61.140
350	162.608	369.859	347.630	7.780	277.774	363.125	-54.192
400	185.342	393.078	351.861	16.487	275.133	375.499	-49.034
450	205.963	416.121	357.723	26.279	272.801	388.187	-45.059
500	224.419	438.795	364.700	37.047	270.741	401.128	-41.905
600	255.484	482.566	380.729	61.102	267.300	427.543	-37.220
700	280.276	523.880	398.259	87.935	264.651	454.473	-33.912
800	300.411	562.665	416.411	117.003	262.697	481.727	-31.453
900	317.045	599.039	434.704	147.901	261.349	509.187	-29.552
1000	330.968	633.184	452.862	180.322	260.524	536.774	-28.038
1100	342.732	665.296	470.730	214.023	260.129	564.424	-26.802
1200	352.740	695.558	488.217	248.810	260.094	592.088	-25.772
1300	361.303	724.139	505.276	284.523	260.333	619.747	-24.901
1400	368.666	751.191	521.884	321.030	260.784	647.382	-24.154
1500	375.026	776.848	538.033	358.223	261.405	674.978	-23.504
1600	380.544	801.232	553.728	396.008	262.136	702.525	-22.935
1700	385.353	824.450	568.975	434.308	262.940	730.014	-22.430
1800	389.560	846.598	583.788	473.058	263.784	757.481	-21.981
1900	393.257	867.762	598.181	512.203	264.651	784.879	-21.577
2000	396.518	888.018	612.170	551.695	265.513	812.241	-21.213
2100	399.406	907.435	625.771	591.494	266.338	839.556	-20.882
2200	401.973	926.076	639.001	631.566	267.124	866.835	-20.581
2300	404.262	943.996	651.874	671.879	267.864	894.075	-20.305
2400	406.311	961.245	664.408	712.410	268.530	921.269	-20.050
2500	408.152	977.870	676.616	753.135	269.125	948.481	-19.817
2600	409.810	993.911	688.513	794.034	269.632	975.624	-19.600
2700	411.308	1009.405	700.112	835.091	270.053	1002.775	-19.399
2800	412.665	1024.389	711.428	876.291	270.377	1029.926	-19.213
2900	413.899	1038.892	722.471	917.620	270.590	1057.043	-19.039
3000	415.023	1052.943	733.254	959.067	270.709	1084.164	-18.877
3100	416.049	1066.568	743.787	1000.622	270.704	1111.256	-18.724
3200	416.989	1079.792	754.081	1042.274	270.588	1138.377	-18.582
3300	417.852	1092.637	764.147	1084.017	270.355	1165.516	-18.448
3400	418.645	1105.123	773.993	1125.842	269.994	1192.635	-18.322
3500	419.376	1117.269	783.628	1167.744	269.506	1219.759	-18.204
3600	420.051	1129.093	793.061	1209.715	268.897	1246.928	-18.092
3700	420.675	1140.611	802.299	1251.752	268.158	1274.127	-17.987
3800	421.254	1151.837	811.350	1293.849	267.275	1301.320	-17.888
3900	421.791	1162.786	820.222	1336.001	266.266	1328.523	-17.793
4000	422.291	1173.472	828.920	1378.206	265.122	1355.804	-17.705
4100	422.757	1183.905	837.451	1420.459	263.831	1383.086	-17.620
4200	423.191	1194.097	845.822	1462.756	262.402	1410.399	-17.541
4300	423.597	1204.060	854.038	1505.096	260.830	1437.713	-17.464
4400	423.977	1213.803	862.104	1547.475	259.119	1465.102	-17.393
4500	424.333	1223.335	870.026	1589.891	257.273	1492.555	-17.325
4600	424.667	1232.665	877.808	1632.341	255.273	1520.048	-17.260
4700	424.981	1241.801	885.456	1674.823	253.123	1547.544	-17.199
4800	425.276	1250.752	892.973	1717.336	250.844	1575.127	-17.141
4900	425.554	1259.524	900.365	1759.878	248.406	1602.710	-17.085
5000	425.816	1268.124	907.634	1802.447	245.845	1630.417	-17.032

3.5. Naphthalene



Other names: Naphthalin
Formula: $C_{10}H_8$
Mass: 128.171 g/mol
CAS Number: 91-20-3
Point Group: D_{2h}

Length: 9.155 Å
Width: 7.395 Å
Breadth: 3.882 Å
L/B Ratio: 1.238

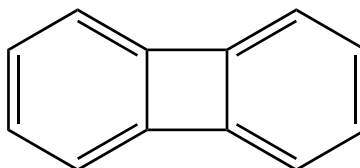
Cartesian coordinates:

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C	2.4198	0.7047	0.0000	C	-2.4183	0.7100	0.0000	H	1.2281	-2.4977	0.0000
C	1.2408	1.3993	0.0000	C	-2.4198	-0.7047	0.0000	H	-1.2282	2.4977	0.0000
C	1.2377	-1.4020	0.0000	C	-1.2408	-1.3993	0.0000	H	-3.3750	1.2423	0.0000
C	-0.0008	-0.7050	0.0000	H	3.3751	-1.2423	0.0000	H	-3.3778	-1.2349	0.0000
C	0.0008	0.7050	0.0000	H	3.3778	1.2349	0.0000	H	-1.2336	-2.4950	0.0000

Table 3.5: Table of thermodynamic data as a function of temperature for Naphthalene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			$\log K_f$
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-20.863	150.914	150.914	∞
100	47.183	248.201	419.374	-17.117	165.265	181.687	-94.902
200	84.845	291.378	344.747	-10.674	157.672	201.090	-52.518
250	109.048	312.874	336.213	-5.835	153.967	212.374	-44.372
298.15	133.325	334.155	334.155	0.000	150.600	223.935	-39.232
300	134.255	334.982	334.157	0.248	150.476	224.389	-39.069
350	158.841	357.540	335.883	7.580	147.302	236.965	-35.364
400	181.799	380.270	340.010	16.104	144.478	249.968	-32.642
450	202.676	402.910	345.743	25.725	141.975	263.306	-30.563
500	221.396	425.251	352.580	36.336	139.758	276.916	-28.929
600	252.958	468.517	368.327	60.114	136.040	304.713	-26.527
700	278.172	509.474	385.594	86.716	133.160	333.066	-24.853
800	298.652	548.001	403.512	115.591	131.013	361.774	-23.621
900	315.564	584.184	421.598	146.328	129.504	390.711	-22.676
1000	329.710	618.186	439.574	178.612	128.542	419.790	-21.927
1100	341.653	650.186	457.280	212.197	128.031	448.946	-21.318
1200	351.808	680.361	474.625	246.883	127.895	478.126	-20.812
1300	360.491	708.873	491.558	282.509	128.047	507.308	-20.383
1400	367.953	735.868	508.053	318.941	128.423	536.473	-20.016
1500	374.396	761.479	524.102	356.066	128.976	565.603	-19.696
1600	379.984	785.825	539.705	393.792	129.648	594.690	-19.414
1700	384.852	809.010	554.870	432.039	130.399	623.721	-19.164
1800	389.110	831.131	569.608	470.742	131.196	652.733	-18.941
1900	392.850	852.272	583.933	509.844	132.020	681.679	-18.740
2000	396.148	872.508	597.859	549.297	132.843	710.591	-18.558
2100	399.069	891.908	611.403	589.061	133.633	739.457	-18.393
2200	401.664	910.534	624.579	629.100	134.386	768.290	-18.241
2300	403.979	928.440	637.404	669.384	135.096	797.086	-18.102
2400	406.050	945.678	649.892	709.887	135.735	825.836	-17.973
2500	407.910	962.292	662.058	750.587	136.305	854.604	-17.856
2600	409.586	978.324	673.915	791.463	136.789	883.306	-17.745
2700	411.100	993.811	685.478	832.499	137.189	912.016	-17.644
2800	412.471	1008.787	696.759	873.679	137.493	940.726	-17.549
2900	413.718	1023.283	707.770	914.989	137.687	969.404	-17.460
3000	414.853	1037.328	718.522	956.418	137.788	998.086	-17.378
3100	415.890	1050.948	729.027	997.956	137.766	1026.740	-17.300
3200	416.840	1064.167	739.294	1039.594	137.636	1055.423	-17.228
3300	417.711	1077.008	749.335	1081.322	137.388	1084.125	-17.160
3400	418.512	1089.490	759.156	1123.133	137.013	1112.807	-17.096
3500	419.250	1101.632	768.769	1165.022	136.512	1141.494	-17.036
3600	419.932	1113.453	778.180	1206.982	135.892	1170.227	-16.979
3700	420.563	1124.967	787.398	1249.007	135.141	1198.991	-16.926
3800	421.147	1136.191	796.429	1291.093	134.247	1227.748	-16.876
3900	421.690	1147.137	805.282	1333.235	133.227	1256.516	-16.829
4000	422.195	1157.820	813.963	1375.429	132.073	1285.362	-16.785
4100	422.665	1168.251	822.477	1417.673	130.773	1314.210	-16.743
4200	423.104	1178.441	830.831	1459.961	129.335	1343.088	-16.703
4300	423.514	1188.402	839.032	1502.293	127.755	1371.968	-16.666
4400	423.898	1198.143	847.083	1544.663	126.035	1400.923	-16.631
4500	424.257	1207.673	854.991	1587.071	124.181	1429.941	-16.598
4600	424.594	1217.002	862.759	1629.514	122.174	1459.000	-16.567
4700	424.911	1226.136	870.394	1671.989	120.017	1488.063	-16.538
4800	425.209	1235.085	877.899	1714.496	117.732	1517.213	-16.510
4900	425.489	1243.856	885.278	1757.031	115.287	1546.362	-16.484
5000	425.754	1252.455	892.536	1799.593	112.719	1575.636	-16.460

3.6. Biphenylene



Other names: Diphenylene
Formula: C₁₂H₈
Mass: 152.19 g/mol
CAS Number: 259-79-0
Point Group: D_{2h}

Length: 10.57 Å
Width: 7.486 Å
Breadth: 3.883 Å
L/B Ratio: 1.412

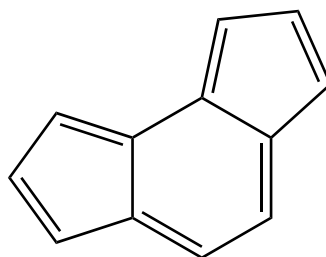
Cartesian coordinates:

C	0.0069	1.3578	0.0123	C	-0.7561	2.6635	0.0287	H	3.3606	-0.5351	-0.0380
C	-0.0403	-0.0179	0.0061	C	-1.9777	3.2976	0.0483	H	3.4133	1.9769	-0.0259
C	1.2180	-0.6811	-0.0125	C	-1.9379	4.7198	0.0561	H	-2.9308	2.7646	0.0573
C	2.4203	0.0216	-0.0236	C	-0.7355	5.4226	0.0452	H	-2.8781	5.2766	0.0711
C	2.4601	1.4439	-0.0170	C	0.5228	4.7594	0.0254	H	-0.7589	6.5152	0.0519
C	1.2385	2.0779	0.0010	H	-0.9729	-0.5861	0.0147	H	1.4554	5.3276	0.0173
C	0.4755	3.3836	0.0175	H	1.2414	-1.7737	-0.0182				

Table 3.6: Table of thermodynamic data as a function of temperature for Biphenylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-24.366	420.571	420.571	∞
100	56.054	261.776	463.834	-20.206	430.758	446.014	-232.969
200	100.366	313.138	375.857	-12.544	423.732	464.031	-121.190
250	128.173	338.482	365.839	-6.839	420.301	474.502	-99.140
298.15	155.896	363.428	363.428	0.000	417.200	485.229	-85.008
300	156.954	364.396	363.431	0.289	417.085	485.651	-84.558
350	184.840	390.705	365.445	8.841	414.189	497.314	-74.218
400	210.724	417.102	370.253	18.740	411.636	509.363	-66.515
450	234.141	443.299	376.917	29.872	409.388	521.715	-60.558
500	255.041	469.072	384.848	42.112	407.404	534.314	-55.818
600	290.065	518.794	403.066	69.437	404.077	560.023	-48.753
700	317.823	565.672	422.982	99.883	401.495	586.230	-43.744
800	340.195	609.623	443.595	132.822	399.570	612.755	-40.008
900	358.540	650.786	464.355	167.788	398.220	639.483	-37.114
1000	373.791	689.375	484.948	204.427	397.367	666.340	-34.805
1100	386.600	725.619	505.196	242.465	396.921	693.266	-32.920
1200	397.445	759.735	525.000	281.682	396.814	720.210	-31.349
1300	406.686	791.923	544.307	321.901	396.961	747.156	-30.020
1400	414.606	822.359	563.091	362.975	397.299	774.086	-28.881
1500	421.427	851.202	581.345	404.785	397.789	800.987	-27.892
1600	427.332	878.593	599.074	447.230	398.370	827.847	-27.026
1700	432.468	904.658	616.289	490.226	399.006	854.658	-26.260
1800	436.954	929.507	633.005	533.702	399.662	881.460	-25.579
1900	440.890	953.239	649.240	577.599	400.323	908.202	-24.968
2000	444.358	975.944	665.012	621.864	400.960	934.921	-24.417
2100	447.425	997.700	680.340	666.457	401.541	961.603	-23.918
2200	450.150	1018.578	695.243	711.338	402.062	988.260	-23.464
2300	452.578	1038.643	709.740	756.477	402.521	1014.894	-23.048
2400	454.750	1057.951	723.849	801.845	402.885	1041.489	-22.667
2500	456.699	1076.555	737.587	847.419	403.159	1068.122	-22.317
2600	458.455	1094.502	750.972	893.179	403.327	1094.693	-21.992
2700	460.040	1111.834	764.018	939.105	403.389	1121.291	-21.692
2800	461.476	1128.591	776.741	985.182	403.334	1147.900	-21.414
2900	462.780	1144.808	789.155	1031.395	403.147	1174.489	-21.154
3000	463.968	1160.518	801.273	1077.734	402.850	1201.097	-20.913
3100	465.053	1175.749	813.108	1124.186	402.406	1227.685	-20.686
3200	466.045	1190.530	824.673	1170.741	401.833	1254.321	-20.474
3300	466.956	1204.885	835.978	1217.392	401.124	1280.994	-20.276
3400	467.794	1218.837	847.034	1264.130	400.266	1307.653	-20.089
3500	468.565	1232.409	857.852	1310.948	399.260	1334.331	-19.913
3600	469.278	1245.619	868.441	1357.841	398.117	1361.078	-19.748
3700	469.937	1258.486	878.809	1404.802	396.822	1387.868	-19.593
3800	470.548	1271.026	888.967	1451.827	395.363	1414.666	-19.446
3900	471.114	1283.256	898.920	1498.910	393.758	1441.484	-19.306
4000	471.642	1295.191	908.679	1546.048	392.000	1468.405	-19.175
4100	472.133	1306.843	918.248	1593.237	390.073	1495.339	-19.050
4200	472.591	1318.226	927.637	1640.474	387.990	1522.318	-18.932
4300	473.019	1329.351	936.850	1687.755	385.743	1549.309	-18.820
4400	473.420	1340.230	945.895	1735.077	383.337	1576.396	-18.714
4500	473.795	1350.874	954.776	1782.438	380.778	1603.565	-18.613
4600	474.147	1361.291	963.501	1829.835	378.043	1630.793	-18.518
4700	474.477	1371.492	972.073	1877.266	375.138	1658.033	-18.427
4800	474.788	1381.484	980.499	1924.730	372.086	1685.384	-18.340
4900	475.081	1391.277	988.783	1972.223	368.851	1712.739	-18.258
5000	475.357	1400.878	996.929	2019.745	365.477	1740.248	-18.180

3.7. as-Indacene



Formula: C₁₂H₈
Mass: 152.192 g/mol
CAS Number: 210-65-1
Point Group: C_{2v}

Length: 10.24 Å
Width: 7.904 Å
Breadth: 3.883 Å
L/B Ratio: 1.296

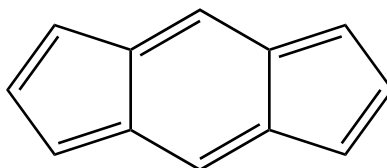
Cartesian coordinates:

C	-0.7154	-0.5848	0.0000	C	2.9854	-0.9184	0.0000	H	1.5107	-2.6404	0.0000
C	0.7142	-0.5864	0.0000	C	2.8355	0.4309	0.0000	H	3.9184	-1.4781	0.0000
C	1.3943	0.7302	0.0000	C	-2.8345	0.4369	0.0000	H	3.6105	1.1938	0.0000
C	0.7288	1.9006	0.0000	C	-2.9874	-0.9121	0.0000	H	-3.6080	1.2014	0.0000
C	-0.7248	1.9021	0.0000	C	-1.6653	-1.5599	0.0000	H	-3.9216	-1.4698	0.0000
C	-1.3928	0.7331	0.0000	H	1.2534	2.8616	0.0000	H	-1.5163	-2.6372	0.0000
C	1.6620	-1.5634	0.0000	H	-1.2473	2.8643	0.0000				

Table 3.7: Table of thermodynamic data as a function of temperature for as-Indacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-24.760	458.355	458.355	∞
100	56.169	266.265	472.740	-20.647	471.472	486.278	-254.001
200	102.685	318.369	382.699	-12.866	464.565	503.818	-131.581
250	131.528	344.347	372.420	-7.018	461.277	514.012	-107.395
298.15	159.926	369.947	369.947	0.000	458.355	524.441	-91.878
300	161.003	370.939	369.950	0.297	458.248	524.851	-91.383
350	189.227	397.902	372.015	9.061	455.564	536.169	-80.017
400	215.178	424.892	376.939	19.181	453.233	547.844	-71.540
450	238.483	451.609	383.755	30.534	451.205	559.794	-64.978
500	259.164	477.828	391.856	42.986	449.433	571.965	-59.752
600	293.611	528.252	410.427	70.695	446.490	596.761	-51.952
700	320.771	575.631	430.681	101.466	444.233	621.997	-46.413
800	342.610	619.941	451.600	134.672	442.576	647.506	-42.277
900	360.507	661.361	472.631	169.857	441.444	673.189	-39.070
1000	375.395	700.138	493.464	206.674	440.769	698.979	-36.510
1100	387.914	736.521	513.924	244.857	440.468	724.822	-34.418
1200	398.528	770.741	533.914	284.193	440.480	750.669	-32.675
1300	407.585	803.008	553.384	324.511	440.726	776.511	-31.200
1400	415.358	833.505	572.313	365.668	441.147	802.329	-29.935
1500	422.063	862.396	590.698	407.547	441.706	828.113	-28.837
1600	427.873	889.825	608.543	450.050	442.345	853.852	-27.875
1700	432.931	915.920	625.863	493.096	443.031	879.538	-27.024
1800	437.355	940.793	642.674	536.615	443.731	905.212	-26.268
1900	441.239	964.546	658.994	580.549	444.428	930.824	-25.590
2000	444.664	987.268	674.844	624.848	445.099	956.412	-24.978
2100	447.695	1009.038	690.243	669.469	445.708	981.961	-24.424
2200	450.389	1029.928	705.212	714.376	446.255	1007.484	-23.920
2300	452.792	1050.002	719.769	759.537	446.736	1032.982	-23.459
2400	454.942	1069.319	733.934	804.926	447.121	1058.441	-23.036
2500	456.872	1087.931	747.724	850.518	447.413	1083.936	-22.647
2600	458.611	1105.884	761.156	896.294	447.597	1109.369	-22.287
2700	460.182	1123.222	774.246	942.235	447.674	1134.829	-21.954
2800	461.606	1139.984	787.011	988.325	447.632	1160.299	-21.645
2900	462.899	1156.205	799.463	1034.552	447.459	1185.748	-21.357
3000	464.077	1171.919	811.618	1080.901	447.172	1211.217	-21.089
3100	465.154	1187.153	823.488	1127.364	446.739	1236.664	-20.837
3200	466.139	1201.937	835.084	1173.929	446.176	1262.159	-20.602
3300	467.043	1216.295	846.420	1220.589	445.476	1287.692	-20.382
3400	467.874	1230.250	857.505	1267.335	444.626	1313.210	-20.175
3500	468.641	1243.824	868.349	1314.161	443.629	1338.747	-19.979
3600	469.348	1257.036	878.963	1361.061	442.493	1364.352	-19.796
3700	470.003	1269.905	889.356	1408.029	441.205	1390.000	-19.623
3800	470.609	1282.447	899.536	1455.060	439.752	1415.656	-19.459
3900	471.173	1294.679	909.512	1502.150	438.153	1441.331	-19.304
4000	471.697	1306.614	919.291	1549.294	436.401	1467.111	-19.158
4100	472.185	1318.268	928.881	1596.488	434.479	1492.902	-19.019
4200	472.640	1329.652	938.288	1643.729	432.401	1518.739	-18.888
4300	473.065	1340.778	947.519	1691.015	430.158	1544.587	-18.763
4400	473.464	1351.659	956.581	1738.342	427.757	1570.531	-18.644
4500	473.837	1362.303	965.479	1785.707	425.202	1596.557	-18.532
4600	474.187	1372.721	974.219	1833.108	422.471	1622.642	-18.425
4700	474.515	1382.923	982.807	1880.543	419.571	1648.739	-18.323
4800	474.825	1392.916	991.247	1928.011	416.522	1674.946	-18.227
4900	475.116	1402.710	999.545	1975.508	413.291	1701.159	-18.134
5000	475.390	1412.311	1007.705	2023.033	409.920	1727.524	-18.047

3.8. s-Indacene



Formula: C₁₂H₈
Mass: 152.192 g/mol
CAS Number: 267-21-0
Point Group: D_{2h}

Length: 11.29 Å
Width: 7.513 Å
Breadth: 3.884 Å
L/B Ratio: 1.503

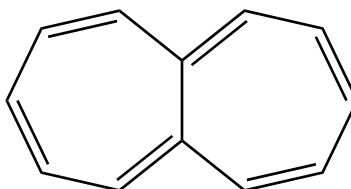
Cartesian coordinates:

C	1.1865	0.7490	0.0000	C	-3.3619	-0.0144	0.0000	H	-2.8351	-2.2133	0.0000
C	-0.0648	1.4645	0.0000	C	-2.6091	1.1194	0.0000	H	-4.4476	-0.0837	0.0000
C	-1.1950	0.7290	0.0000	C	2.6091	-1.1194	0.0000	H	-2.9525	2.1515	0.0000
C	-1.1865	-0.7490	0.0000	C	3.3619	0.0144	0.0000	H	2.8351	2.2133	0.0000
C	0.0648	-1.4645	0.0000	C	2.4812	1.1844	0.0000	H	4.4476	0.0837	0.0000
C	1.1950	-0.7290	0.0000	H	-0.0654	2.5589	0.0000	H	2.9525	-2.1515	0.0000
C	-2.4812	-1.1844	0.0000	H	0.0654	-2.5589	0.0000				

Table 3.8: Table of thermodynamic data as a function of temperature for s-Indacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-24.892	417.686	417.686	∞
100	56.010	260.278	468.185	-20.791	430.660	446.065	-232.996
200	103.579	312.743	377.498	-12.951	423.811	464.189	-121.231
250	132.391	338.918	367.154	-7.059	420.567	474.660	-99.173
298.15	160.766	364.667	364.667	0.000	417.686	485.346	-85.029
300	161.843	365.665	364.670	0.298	417.581	485.766	-84.578
350	190.092	392.759	366.745	9.105	414.939	497.345	-74.223
400	216.093	419.867	371.693	19.270	412.652	509.273	-66.503
450	239.448	446.694	378.540	30.670	410.672	521.472	-60.530
500	260.167	473.017	386.676	43.171	408.949	533.886	-55.774
600	294.636	523.627	405.325	70.982	406.108	559.154	-48.678
700	321.764	571.163	425.658	101.854	403.952	584.844	-43.641
800	343.540	615.601	446.655	135.157	402.391	610.794	-39.880
900	361.363	657.127	467.760	170.430	401.349	636.905	-36.964
1000	376.175	695.990	488.661	207.329	400.756	663.114	-34.637
1100	388.622	732.444	509.183	245.587	400.529	689.367	-32.735
1200	399.169	766.723	529.231	284.990	400.609	715.620	-31.149
1300	408.167	799.038	548.754	325.369	400.915	741.861	-29.808
1400	415.886	829.576	567.732	366.581	401.392	768.074	-28.657
1500	422.542	858.502	586.161	408.511	402.001	794.248	-27.658
1600	428.310	885.961	604.048	451.060	402.687	820.375	-26.782
1700	433.331	912.081	621.406	494.148	403.414	846.447	-26.008
1800	437.720	936.976	638.251	537.705	404.152	872.504	-25.319
1900	441.575	960.748	654.604	581.674	404.885	898.497	-24.701
2000	444.973	983.486	670.484	626.005	405.587	924.463	-24.144
2100	447.981	1005.271	685.911	670.656	406.226	950.389	-23.639
2200	450.653	1026.174	700.906	715.590	406.800	976.289	-23.180
2300	453.037	1046.260	715.487	760.777	407.307	1002.162	-22.759
2400	455.169	1065.587	729.674	806.189	407.715	1027.994	-22.373
2500	457.084	1084.207	743.486	851.803	408.030	1053.862	-22.019
2600	458.809	1102.168	756.938	897.599	408.234	1079.667	-21.690
2700	460.367	1119.514	770.047	943.560	408.330	1105.498	-21.387
2800	461.779	1136.282	782.829	989.668	408.306	1131.339	-21.105
2900	463.062	1152.509	795.298	1035.911	408.150	1157.158	-20.842
3000	464.230	1168.228	807.469	1082.277	407.879	1182.996	-20.597
3100	465.298	1183.467	819.353	1128.754	407.460	1208.812	-20.368
3200	466.275	1198.256	830.964	1175.333	406.912	1234.676	-20.154
3300	467.172	1212.618	842.313	1222.006	406.225	1260.576	-19.953
3400	467.996	1226.577	853.410	1268.765	405.387	1286.462	-19.764
3500	468.756	1240.154	864.267	1315.603	404.402	1312.366	-19.586
3600	469.457	1253.369	874.893	1362.514	403.277	1338.337	-19.418
3700	470.107	1266.241	885.296	1409.493	401.999	1364.353	-19.261
3800	470.708	1278.786	895.487	1456.534	400.556	1390.375	-19.112
3900	471.267	1291.020	905.473	1503.633	398.968	1416.416	-18.970
4000	471.786	1302.958	915.261	1550.786	397.224	1442.561	-18.838
4100	472.270	1314.613	924.860	1597.989	395.312	1468.719	-18.711
4200	472.722	1325.999	934.276	1645.239	393.241	1494.920	-18.592
4300	473.143	1337.128	943.516	1692.532	391.007	1521.134	-18.478
4400	473.538	1348.010	952.585	1739.867	388.613	1547.442	-18.370
4500	473.908	1358.656	961.491	1787.239	386.066	1573.833	-18.268
4600	474.255	1369.076	970.239	1834.648	383.342	1600.284	-18.171
4700	474.581	1379.278	978.834	1882.090	380.448	1626.745	-18.079
4800	474.888	1389.273	987.281	1929.563	377.406	1653.316	-17.991
4900	475.176	1399.068	995.585	1977.067	374.181	1679.893	-17.908
5000	475.449	1408.671	1003.751	2024.598	370.816	1706.623	-17.829

3.9. Heptalene



Formula: C₁₂H₁₀
Mass: 154.21 g/mol
CAS Number: 257-24-9
Point Group: C₂

Length: 10.47 Å
Width: 7.292 Å
Breadth: 5.140 Å
L/B Ratio: 1.436

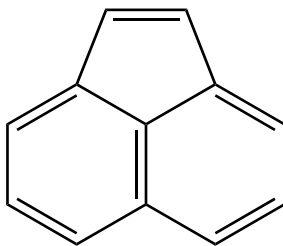
Cartesian coordinates:

C	0.0581	1.2616	0.1477	C	0.6045	3.6866	2.0802	H	2.7866	2.7703	-1.2227
C	0.0472	-0.0829	-0.1185	C	-0.7500	3.5800	2.1612	H	2.4536	3.6272	0.9981
C	1.1321	-0.9780	-0.4381	C	-1.5973	2.8915	1.2120	H	1.0993	4.3212	2.8232
C	2.3549	-0.6569	-0.9427	C	-1.2503	1.9326	0.3184	H	-1.2592	4.1267	2.9602
C	2.8035	0.6781	-1.2743	H	-0.9373	-0.5607	-0.0614	H	-2.6542	3.1810	1.2260
C	2.3173	1.8624	-0.8278	H	0.9030	-2.0433	-0.3280	H	-2.0454	1.5510	-0.3319
C	1.2739	2.1034	0.1939	H	3.0323	-1.4756	-1.2022				
C	1.4732	3.1420	1.0657	H	3.6477	0.7328	-1.9709				

Table 3.9: Table of thermodynamic data as a function of temperature for Heptalene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-27.463	421.344	421.344	∞
100	63.973	275.807	504.734	-22.893	437.683	461.608	-241.114
200	114.545	334.883	405.290	-14.081	429.112	488.945	-127.697
250	143.923	363.570	394.074	-7.626	425.036	504.375	-105.381
298.15	172.799	391.392	391.392	0.000	421.344	519.998	-91.100
300	173.898	392.464	391.395	0.321	421.208	520.610	-90.644
350	202.884	421.468	393.620	9.747	417.737	537.458	-80.210
400	229.885	450.348	398.909	20.576	414.657	554.772	-72.444
450	254.463	478.868	406.213	32.695	411.935	572.452	-66.447
500	276.560	506.843	414.882	45.981	409.534	590.427	-61.680
600	314.027	560.704	434.739	75.579	405.552	626.998	-54.584
700	344.202	611.459	456.397	108.543	402.550	664.159	-49.559
800	368.882	659.085	478.788	144.237	400.427	701.681	-45.814
900	389.373	703.752	501.329	182.180	399.080	739.420	-42.914
1000	406.578	745.693	523.690	222.002	398.406	777.278	-40.600
1100	421.142	785.146	545.683	263.408	398.289	815.179	-38.709
1200	433.546	822.336	567.203	306.159	398.638	853.061	-37.132
1300	444.164	857.468	588.193	350.058	399.344	890.905	-35.796
1400	453.295	890.727	608.625	394.942	400.328	928.686	-34.649
1500	461.183	922.276	628.492	440.676	401.534	966.388	-33.652
1600	468.026	952.264	647.799	487.144	402.887	1004.001	-32.777
1700	473.987	980.821	666.555	534.251	404.340	1041.513	-32.001
1800	479.201	1008.064	684.777	581.917	405.851	1078.969	-31.310
1900	483.782	1034.098	702.482	630.071	407.397	1116.315	-30.689
2000	487.822	1059.018	719.691	678.655	408.944	1153.592	-30.128
2100	491.398	1082.907	736.422	727.619	410.450	1190.785	-29.619
2200	494.576	1105.842	752.696	776.921	411.913	1227.911	-29.154
2300	497.410	1127.890	768.532	826.523	413.324	1264.967	-28.728
2400	499.946	1149.114	783.951	876.393	414.649	1301.945	-28.336
2500	502.223	1169.570	798.969	926.504	415.890	1338.922	-27.975
2600	504.275	1189.308	813.604	976.830	417.026	1375.796	-27.640
2700	506.128	1208.375	827.874	1027.352	418.060	1412.658	-27.329
2800	507.807	1226.813	841.795	1078.050	418.977	1449.501	-27.040
2900	509.332	1244.659	855.381	1128.908	419.761	1486.284	-26.770
3000	510.722	1261.950	868.646	1179.912	420.432	1523.054	-26.518
3100	511.991	1278.718	881.605	1231.049	420.952	1559.772	-26.281
3200	513.153	1294.991	894.271	1282.307	421.341	1596.507	-26.060
3300	514.219	1310.799	906.654	1333.676	421.586	1633.248	-25.852
3400	515.199	1326.164	918.768	1385.148	421.677	1669.949	-25.655
3500	516.102	1341.112	930.622	1436.713	421.614	1706.640	-25.470
3600	516.937	1355.663	942.228	1488.366	421.406	1743.370	-25.295
3700	517.708	1369.837	953.594	1540.098	421.038	1780.123	-25.130
3800	518.423	1383.653	964.730	1591.905	420.496	1816.852	-24.974
3900	519.087	1397.128	975.645	1643.781	419.801	1853.582	-24.825
4000	519.705	1410.278	986.348	1695.721	418.943	1890.392	-24.685
4100	520.280	1423.118	996.845	1747.721	417.906	1927.190	-24.552
4200	520.817	1435.662	1007.144	1799.776	416.702	1964.012	-24.426
4300	521.318	1447.923	1017.252	1851.883	415.323	2000.824	-24.305
4400	521.787	1459.913	1027.177	1904.039	413.776	2037.713	-24.190
4500	522.227	1471.644	1036.924	1956.240	412.064	2074.668	-24.082
4600	522.640	1483.127	1046.500	2008.483	410.165	2111.660	-23.978
4700	523.027	1494.371	1055.910	2060.767	408.085	2148.645	-23.879
4800	523.391	1505.386	1065.160	2113.088	405.847	2185.723	-23.785
4900	523.735	1516.182	1074.254	2165.444	403.415	2222.791	-23.695
5000	524.058	1526.766	1083.199	2217.834	400.834	2259.999	-23.610

3.10. Acenaphthylene



Other names: Acenaphthalene
Cyclopenta[de]naphthalene

Formula: C₁₂H₈
Mass: 152.192 g/mol
CAS Number: 208-96-8
Point Group: C_{2v}

Length: 9.199 Å
Width: 8.572 Å
Breadth: 3.883 Å
L/B Ratio: 1.073

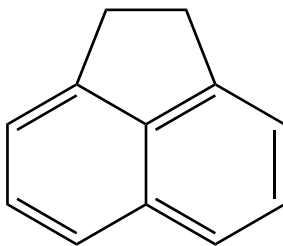
Cartesian coordinates:

C	-1.1674	-0.9456	0.0000	C	2.4145	1.1133	0.0000	H	3.3303	-0.8711	0.0000
C	0.0005	-0.1247	0.0000	C	2.3906	-0.3108	0.0000	H	3.3934	1.6055	0.0000
C	-0.0050	1.2617	0.0000	C	1.1748	-0.9363	0.0000	H	1.3368	2.9773	0.0000
C	-1.2901	1.8738	0.0000	C	0.6903	-2.3280	0.0000	H	-1.3603	2.9667	0.0000
C	-2.4232	1.0943	0.0000	C	-0.6719	-2.3333	0.0000	H	-3.4059	1.5789	0.0000
C	-2.3881	-0.3296	0.0000	H	1.3521	-3.1916	0.0000	H	-3.3233	-0.8974	0.0000
C	1.2754	1.8839	0.0000	H	-1.3270	-3.2020	0.0000				

Table 3.10: Table of thermodynamic data as a function of temperature for Acenaphthylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-23.180	269.991	269.991	∞
100	50.537	261.512	454.905	-19.339	277.625	292.907	-152.996
200	96.038	309.268	370.220	-12.190	270.086	311.158	-81.265
250	124.625	333.735	360.461	-6.681	266.459	321.847	-67.245
298.15	152.859	358.103	358.103	0.000	263.200	332.817	-58.307
300	153.934	359.052	358.106	0.284	263.080	333.249	-58.023
350	182.193	384.925	360.085	8.694	260.042	345.190	-51.516
400	208.374	410.989	364.818	18.468	257.364	357.537	-46.689
450	232.046	436.924	371.392	29.489	255.005	370.202	-42.971
500	253.173	462.487	379.227	41.630	252.922	383.124	-40.024
600	288.575	511.904	397.257	68.788	249.428	409.508	-35.650
700	316.623	558.575	417.003	99.100	246.712	436.416	-32.565
800	339.215	602.381	437.467	131.931	244.679	463.658	-30.273
900	357.726	643.438	458.096	166.808	243.240	491.116	-28.503
1000	373.105	681.949	478.576	203.372	242.312	518.712	-27.094
1100	386.014	718.132	498.726	241.347	241.803	546.384	-25.945
1200	396.939	752.201	518.444	280.509	241.641	574.078	-24.988
1300	406.245	784.350	537.673	320.680	241.740	601.780	-24.179
1400	414.217	814.756	556.389	361.714	242.038	629.469	-23.485
1500	421.082	843.574	574.582	403.487	242.491	657.131	-22.883
1600	427.024	870.944	592.257	445.899	243.039	684.755	-22.354
1700	432.191	896.991	609.422	488.866	243.646	712.332	-21.887
1800	436.704	921.825	626.094	532.316	244.276	739.901	-21.471
1900	440.663	945.544	642.287	576.188	244.912	767.412	-21.097
2000	444.151	968.238	658.022	620.433	245.529	794.901	-20.760
2100	447.237	989.984	673.315	665.005	246.089	822.354	-20.455
2200	449.976	1010.854	688.187	709.869	246.593	849.784	-20.176
2300	452.418	1030.911	702.655	754.991	247.035	877.190	-19.921
2400	454.602	1050.213	716.737	800.344	247.384	904.559	-19.687
2500	456.563	1068.811	730.450	845.904	247.644	931.965	-19.472
2600	458.327	1086.753	743.811	891.650	247.798	959.311	-19.272
2700	459.921	1104.081	756.835	937.563	247.847	986.684	-19.088
2800	461.365	1120.834	769.538	983.629	247.781	1014.069	-18.917
2900	462.677	1137.047	781.932	1029.832	247.584	1041.434	-18.758
3000	463.871	1152.753	794.033	1076.160	247.276	1068.818	-18.609
3100	464.962	1167.981	805.851	1122.603	246.823	1096.183	-18.470
3200	465.960	1182.759	817.400	1169.150	246.242	1123.596	-18.340
3300	466.875	1197.111	828.690	1215.792	245.524	1151.046	-18.219
3400	467.717	1211.062	839.732	1262.522	244.658	1178.483	-18.105
3500	468.493	1224.631	850.536	1309.333	243.645	1205.939	-17.997
3600	469.209	1237.839	861.112	1356.219	242.495	1233.463	-17.897
3700	469.872	1250.704	871.468	1403.173	241.193	1261.031	-17.802
3800	470.486	1263.243	881.614	1450.192	239.728	1288.607	-17.713
3900	471.056	1275.472	891.556	1497.269	238.117	1316.203	-17.628
4000	471.586	1287.404	901.304	1544.401	236.353	1343.904	-17.549
4100	472.080	1299.055	910.864	1591.585	234.421	1371.616	-17.474
4200	472.540	1310.437	920.242	1638.816	232.332	1399.374	-17.403
4300	472.971	1321.561	929.447	1686.092	230.080	1427.144	-17.336
4400	473.373	1332.439	938.482	1733.409	227.669	1455.010	-17.273
4500	473.750	1343.081	947.356	1780.766	225.106	1482.958	-17.213
4600	474.104	1353.498	956.072	1828.159	222.367	1510.966	-17.157
4700	474.437	1363.698	964.637	1875.586	219.458	1538.985	-17.104
4800	474.749	1373.689	973.055	1923.045	216.401	1567.115	-17.053
4900	475.044	1383.481	981.331	1970.535	213.163	1595.250	-17.005
5000	475.321	1393.081	989.471	2018.054	209.786	1623.538	-16.961

3.11. Acenaphthene



Other names: 1,2-Dihydroacenaphthylene
1,8-Ethylenenaphthalene

Formula: $C_{12}H_{10}$

Mass: 154.208 g/mol

CAS Number: 83-32-9

Point Group: C_{2v}

Length: 9.191 Å

Width: 8.492 Å

Breadth: 4.169 Å

L/B Ratio: 1.082

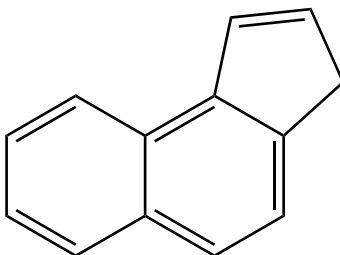
Cartesian coordinates:

C	-2.3954	-0.2346	0.0000	C	2.3883	-0.2986	0.0000	H	3.3200	-0.8717	0.0000
C	-1.1912	-0.8808	0.0000	C	1.1671	-0.9124	0.0000	H	3.4172	1.6044	0.0000
C	-0.0014	-0.1064	0.0000	C	0.7466	-2.3505	0.0000	H	1.3667	2.9929	0.0000
C	0.0172	1.2861	0.0000	C	-0.8093	-2.3297	0.0000	H	-1.2862	3.0284	0.0000
C	-1.2489	1.9341	0.0000	H	1.1452	-2.8788	0.8847	H	-3.3731	1.6953	0.0000
C	-2.4022	1.1878	0.0000	H	1.1452	-2.8788	-0.8847	H	-3.3421	-0.7826	0.0000
C	1.3003	1.8999	0.0000	H	-1.2219	-2.8471	0.8848				
C	2.4332	1.1231	0.0000	H	-1.2219	-2.8471	-0.8848				

Table 3.11: Table of thermodynamic data as a function of temperature for Acenaphthene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-24.997	160.742	160.742	∞
100	57.059	268.632	476.368	-20.774	176.458	201.101	-105.042
200	103.022	321.078	385.807	-12.946	166.904	229.497	-59.937
250	132.232	347.159	375.457	-7.075	162.243	245.686	-51.332
298.15	161.681	372.962	372.962	0.000	158.000	262.149	-45.926
300	162.813	373.966	372.965	0.300	157.843	262.795	-45.756
350	192.837	401.335	375.058	9.197	153.843	280.611	-41.878
400	221.039	428.951	380.068	19.553	150.290	298.964	-39.040
450	246.806	456.498	387.032	31.260	147.156	317.739	-36.881
500	269.995	483.724	395.343	44.191	144.401	336.853	-35.190
600	309.254	536.555	414.510	73.227	139.856	375.791	-32.715
700	340.735	586.677	435.560	105.782	136.445	415.401	-30.997
800	366.350	633.905	457.431	141.179	134.025	455.423	-29.735
900	387.508	678.314	479.532	178.904	132.460	495.694	-28.769
1000	405.193	720.085	501.520	218.565	131.625	536.104	-28.003
1100	420.105	759.423	523.195	259.851	131.388	576.572	-27.379
1200	432.762	796.534	544.442	302.511	131.646	617.031	-26.858
1300	443.567	831.612	565.195	346.341	132.283	657.458	-26.416
1400	452.838	864.831	585.422	391.173	133.215	697.827	-26.036
1500	460.831	896.353	605.109	436.867	134.381	738.120	-25.703
1600	467.752	926.321	624.256	483.304	135.703	778.326	-25.409
1700	473.774	954.863	642.871	530.387	137.132	818.433	-25.147
1800	479.035	982.095	660.966	578.033	138.624	858.485	-24.912
1900	483.652	1008.122	678.557	626.173	140.156	898.429	-24.699
2000	487.720	1033.036	695.663	674.746	141.691	938.303	-24.505
2100	491.319	1056.920	712.301	723.701	143.188	978.095	-24.328
2200	494.514	1079.852	728.490	772.996	144.644	1017.820	-24.166
2300	497.362	1101.898	744.249	822.592	146.049	1057.476	-24.016
2400	499.910	1123.120	759.596	872.458	147.370	1097.052	-23.876
2500	502.196	1143.575	774.548	922.566	148.608	1136.629	-23.748
2600	504.254	1163.312	789.123	972.890	149.742	1176.103	-23.628
2700	506.113	1182.378	803.337	1023.410	150.774	1215.565	-23.516
2800	507.797	1200.815	817.206	1074.107	151.690	1255.007	-23.412
2900	509.326	1218.661	830.743	1124.964	152.473	1294.390	-23.314
3000	510.719	1235.952	843.963	1175.967	153.143	1333.760	-23.222
3100	511.990	1252.720	856.880	1227.104	153.664	1373.078	-23.136
3200	513.154	1268.993	869.505	1278.362	154.052	1412.412	-23.055
3300	514.222	1284.800	881.852	1329.731	154.297	1451.753	-22.979
3400	515.203	1300.166	893.930	1381.203	154.389	1491.054	-22.907
3500	516.108	1315.114	905.751	1432.769	154.326	1530.344	-22.839
3600	516.943	1329.665	917.325	1484.422	154.118	1569.674	-22.775
3700	517.715	1343.839	928.662	1536.156	153.752	1609.027	-22.715
3800	518.431	1357.656	939.770	1587.964	153.211	1648.356	-22.658
3900	519.095	1371.131	950.659	1639.840	152.516	1687.686	-22.604
4000	519.713	1384.281	961.336	1691.781	151.659	1727.095	-22.553
4100	520.289	1397.121	971.809	1743.782	150.623	1766.493	-22.505
4200	520.825	1409.665	982.085	1795.838	149.420	1805.914	-22.459
4300	521.327	1421.927	992.172	1847.945	148.041	1845.326	-22.416
4400	521.796	1433.917	1002.076	1900.102	146.495	1884.815	-22.375
4500	522.236	1445.648	1011.803	1952.304	144.784	1924.370	-22.337
4600	522.648	1457.131	1021.360	2004.548	142.886	1963.961	-22.301
4700	523.036	1468.376	1030.752	2056.833	140.807	2003.546	-22.266
4800	523.400	1479.391	1039.984	2109.154	138.569	2043.224	-22.234
4900	523.743	1490.187	1049.062	2161.512	136.139	2082.890	-22.203
5000	524.066	1500.771	1057.991	2213.902	133.558	2122.698	-22.175

3.12. 3*H*-Benz[*e*]indene



Other names: 3*H*- α -Naphthindene
Formula: C₁₃H₁₀
Mass: 166.219 g/mol
CAS Number: 232-55-3
Point Group: C_s

Length: 10.87 Å
Width: 7.956 Å
Breadth: 4.174 Å
L/B Ratio: 1.366

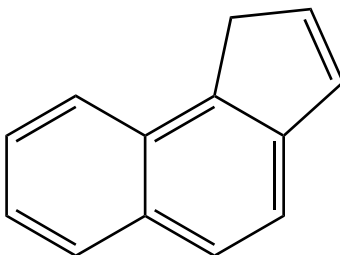
Cartesian coordinates:

C	-2.5142	-1.0094	0.0000	C	1.0982	-1.9450	0.0000	H	3.9589	1.8418	0.0000
C	-1.0973	-0.8891	0.0000	C	-0.2708	-2.0470	0.0000	H	-0.7510	-3.0323	0.0000
C	-0.5211	0.4031	0.0000	C	3.1242	-0.2767	0.0000	H	1.7370	-2.8334	0.0000
C	-1.3648	1.5451	0.0000	C	3.0611	1.2273	0.0000	H	-0.9070	2.5408	0.0000
C	-2.7252	1.3971	0.0000	C	1.7774	1.6521	0.0000	H	-3.3799	2.2746	0.0000
C	-3.3053	0.1071	0.0000	H	1.4203	2.6810	-0.0000	H	-4.3963	0.0150	0.0000
C	0.8916	0.4877	0.0000	H	3.6553	-0.6626	-0.8892	H	-2.9598	-2.0106	0.0000
C	1.6755	-0.6649	0.0000	H	3.6553	-0.6626	0.8892				

Table 3.12: Table of thermodynamic data as a function of temperature for 3*H*-Benz[*e*]indene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-26.876	234.672	234.672	∞
100	60.619	278.664	504.386	-22.572	252.323	276.057	-144.195
200	112.331	335.485	405.887	-14.080	243.106	303.435	-79.247
250	143.878	363.898	394.636	-7.685	238.674	319.030	-66.656
298.15	175.321	391.927	391.927	0.000	234.672	334.878	-58.668
300	176.523	393.015	391.930	0.325	234.524	335.499	-58.414
350	208.281	422.632	394.197	9.952	230.783	352.632	-52.626
400	237.895	452.406	399.612	21.117	227.487	370.264	-48.351
450	264.800	482.007	407.126	33.697	224.597	388.288	-45.070
500	288.903	511.178	416.077	47.551	222.067	406.624	-42.479
600	329.490	567.582	436.667	78.549	217.906	443.946	-38.648
700	361.853	620.894	459.216	113.175	214.794	481.882	-35.958
800	388.078	670.984	482.589	150.715	212.596	520.192	-33.964
900	409.682	717.980	506.161	190.637	211.193	558.726	-32.427
1000	427.708	762.105	529.572	232.533	210.470	597.386	-31.204
1100	442.892	803.602	552.616	276.084	210.304	636.094	-30.205
1200	455.776	842.706	575.177	321.035	210.602	674.788	-29.372
1300	466.772	879.633	597.190	367.176	211.251	713.448	-28.666
1400	476.208	914.579	618.624	414.337	212.172	752.049	-28.059
1500	484.343	947.718	639.468	462.375	213.308	790.577	-27.530
1600	491.391	979.207	659.726	511.170	214.583	829.019	-27.064
1700	497.523	1009.186	679.408	560.622	215.949	867.366	-26.650
1800	502.883	1037.778	698.529	610.649	217.364	905.664	-26.281
1900	507.587	1065.097	717.109	661.177	218.806	943.856	-25.948
2000	511.733	1091.240	735.166	712.147	220.239	981.985	-25.646
2100	515.401	1116.298	752.723	763.508	221.623	1020.036	-25.371
2200	518.659	1140.351	769.799	815.214	222.953	1058.026	-25.120
2300	521.564	1163.472	786.416	867.228	224.223	1095.953	-24.889
2400	524.162	1185.725	802.593	919.516	225.396	1133.805	-24.676
2500	526.495	1207.171	818.350	972.051	226.476	1171.667	-24.480
2600	528.595	1227.862	833.705	1024.808	227.442	1209.429	-24.297
2700	530.492	1247.847	848.676	1077.764	228.296	1247.189	-24.128
2800	532.210	1267.172	863.279	1130.900	229.024	1284.936	-23.970
2900	533.772	1285.875	877.530	1184.200	229.608	1322.629	-23.823
3000	535.193	1303.995	891.445	1237.650	230.071	1360.316	-23.685
3100	536.492	1321.566	905.038	1291.235	230.372	1397.957	-23.555
3200	537.680	1338.618	918.323	1344.944	230.531	1435.623	-23.434
3300	538.771	1355.180	931.311	1398.768	230.539	1473.306	-23.320
3400	539.773	1371.279	944.016	1452.696	230.381	1510.951	-23.212
3500	540.697	1386.939	956.448	1506.720	230.060	1548.593	-23.111
3600	541.550	1402.183	968.619	1560.833	229.583	1586.286	-23.016
3700	542.339	1417.032	980.538	1615.028	228.938	1624.009	-22.926
3800	543.070	1431.505	992.216	1669.298	228.108	1661.715	-22.841
3900	543.749	1445.620	1003.661	1723.640	227.116	1699.426	-22.761
4000	544.380	1459.395	1014.883	1778.047	225.950	1737.231	-22.685
4100	544.968	1472.844	1025.890	1832.514	224.595	1775.029	-22.614
4200	545.516	1485.983	1036.689	1887.039	223.064	1812.858	-22.546
4300	546.029	1498.826	1047.287	1941.616	221.347	1850.682	-22.481
4400	546.508	1511.384	1057.693	1996.243	219.452	1888.595	-22.420
4500	546.958	1523.671	1067.912	2050.917	217.384	1926.583	-22.363
4600	547.379	1535.697	1077.951	2105.634	215.118	1964.617	-22.308
4700	547.775	1547.474	1087.816	2160.392	212.660	2002.648	-22.256
4800	548.147	1559.010	1097.512	2215.188	210.035	2040.784	-22.208
4900	548.498	1570.316	1107.047	2270.021	207.206	2078.912	-22.161
5000	548.829	1581.401	1116.423	2324.887	204.218	2117.195	-22.118

3.13. 1*H*-Benz[*e*]indene



Other names: 1*H*- α -Naphthindene

Formula: C₁₃H₁₀

Mass: 166.219 g/mol

CAS Number: 232-54-2

Point Group: C_s

Length: 10.96 Å

Width: 7.963 Å

Breadth: 4.176 Å

L/B Ratio: 1.376

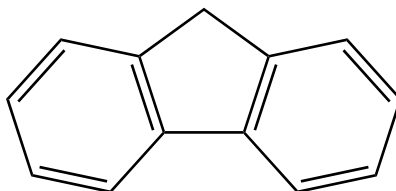
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C	-1.7570	1.7164	-0.0028	C	0.5232	0.3860	-0.0003	H	-4.0337	1.7567	-0.0024
C	-3.0924	-0.2206	0.0008	C	1.3847	1.5155	0.0016	H	0.6941	-3.0525	-0.0018
C	-3.1441	1.1302	-0.0015	C	2.7420	1.3459	0.0023	H	-1.7924	-2.8085	0.0012
C	-1.6910	-0.6400	0.0012	C	3.3009	0.0460	0.0008	H	0.9376	2.5160	0.0029
C	-0.8843	0.4958	-0.0007	C	2.4924	-1.0579	-0.0006	H	3.4114	2.2123	0.0039
C	0.2305	-2.0593	-0.0006	H	-1.5816	2.3476	-0.8936	H	4.3903	-0.0630	0.0009
C	-1.1354	-1.9334	0.0008	H	-1.5813	2.3520	0.8847	H	2.9219	-2.0662	-0.0016
C	1.0776	-0.9157	-0.0008	H	-3.9265	-0.9200	0.0032				

Table 3.13: Table of thermodynamic data as a function of temperature for 1*H*-Benz[*e*]indene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-26.863	234.903	234.903	∞
100	60.613	278.557	504.199	-22.564	252.562	276.308	-144.325
200	112.285	335.360	405.736	-14.075	243.343	303.696	-79.316
250	143.825	363.762	394.489	-7.682	238.908	319.299	-66.712
298.15	175.261	391.781	391.781	0.000	234.903	335.153	-58.716
300	176.463	392.869	391.785	0.325	234.756	335.775	-58.462
350	208.214	422.477	394.050	9.949	231.012	352.915	-52.669
400	237.825	452.241	399.464	21.111	227.712	370.555	-48.389
450	264.728	481.833	406.975	33.686	224.819	388.587	-45.105
500	288.832	510.997	415.924	47.537	222.285	406.932	-42.511
600	329.426	567.388	436.508	78.528	218.117	444.273	-38.677
700	361.799	620.692	459.051	113.148	214.999	482.229	-35.984
800	388.036	670.775	482.420	150.684	212.796	520.559	-33.988
900	409.650	717.766	505.986	190.602	211.389	559.115	-32.450
1000	427.684	761.888	529.393	232.495	210.663	597.796	-31.225
1100	442.875	803.384	552.434	276.044	210.495	636.526	-30.225
1200	455.764	842.486	574.992	320.993	210.792	675.242	-29.392
1300	466.764	879.413	597.002	367.134	211.440	713.923	-28.685
1400	476.203	914.358	618.433	414.294	212.361	752.547	-28.077
1500	484.340	947.497	639.276	462.331	213.496	791.096	-27.548
1600	491.389	978.986	659.532	511.126	214.770	829.561	-27.082
1700	497.523	1008.964	679.212	560.579	216.137	867.930	-26.668
1800	502.883	1037.557	698.332	610.605	217.552	906.250	-26.298
1900	507.588	1064.875	716.910	661.134	218.994	944.464	-25.965
2000	511.735	1091.019	734.967	712.104	220.427	982.616	-25.663
2100	515.403	1116.077	752.522	763.465	221.811	1020.689	-25.388
2200	518.662	1140.130	769.598	815.171	223.141	1058.701	-25.136
2300	521.567	1163.251	786.214	867.185	224.411	1096.650	-24.905
2400	524.165	1185.505	802.390	919.474	225.585	1134.524	-24.692
2500	526.497	1206.950	818.146	972.009	226.666	1172.408	-24.496
2600	528.598	1227.641	833.501	1024.766	227.632	1210.192	-24.313
2700	530.495	1247.627	848.471	1077.722	228.486	1247.974	-24.143
2800	532.213	1266.951	863.073	1130.859	229.214	1285.742	-23.985
2900	533.774	1285.655	877.324	1184.159	229.799	1323.458	-23.838
3000	535.196	1303.775	891.239	1237.609	230.261	1361.167	-23.700
3100	536.494	1321.346	904.831	1291.195	230.563	1398.830	-23.570
3200	537.683	1338.398	918.115	1344.904	230.723	1436.518	-23.448
3300	538.773	1354.960	931.103	1398.728	230.730	1474.223	-23.335
3400	539.775	1371.059	943.807	1452.656	230.573	1511.890	-23.227
3500	540.699	1386.719	956.239	1506.680	230.252	1549.554	-23.125
3600	541.552	1401.964	968.410	1560.793	229.776	1587.269	-23.030
3700	542.341	1416.812	980.329	1614.989	229.131	1625.014	-22.941
3800	543.072	1431.285	992.007	1669.260	228.301	1662.742	-22.856
3900	543.751	1445.401	1003.452	1723.601	227.308	1700.475	-22.775
4000	544.382	1459.176	1014.674	1778.008	226.143	1738.301	-22.699
4100	544.970	1472.625	1025.680	1832.476	224.788	1776.121	-22.628
4200	545.518	1485.764	1036.478	1887.001	223.257	1813.973	-22.560
4300	546.031	1498.607	1047.077	1941.578	221.541	1851.819	-22.495
4400	546.510	1511.165	1057.482	1996.206	219.646	1889.754	-22.434
4500	546.959	1523.452	1067.701	2050.879	217.578	1927.763	-22.376
4600	547.381	1535.478	1077.740	2105.597	215.312	1965.819	-22.322
4700	547.777	1547.254	1087.604	2160.355	212.854	2003.872	-22.270
4800	548.149	1558.791	1097.301	2215.151	210.230	2042.030	-22.221
4900	548.499	1570.097	1106.835	2269.984	207.400	2080.180	-22.175
5000	548.830	1581.182	1116.211	2324.850	204.413	2118.485	-22.131

3.14. Fluorene



Other names: o-Biphenylenemethane
Diphenylenemethane
H-Fluorene
2,2'-Methylenebiphenyl
2,3-Benzidene
o-Biphenylmethane

Formula: C₁₃H₁₀
Mass: 166.219 g/mol
CAS Number: 86-73-7
Point Group: C_{2v}

Length: 11.42 Å
Width: 7.506 Å
Breadth: 4.176 Å
L/B Ratio: 1.521

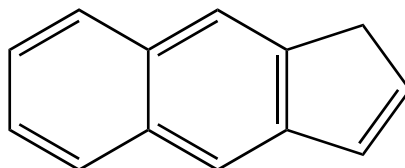
Cartesian coordinates:

C	0.0005	-1.8277	0.0000	C	-0.7307	0.4538	0.0000	H	4.5095	-0.3366	0.0000
C	0.7305	0.4542	0.0000	C	-1.6361	1.5011	0.0000	H	3.7306	2.0112	0.0000
C	1.1751	-0.8896	0.0000	C	-2.9987	1.1956	0.0000	H	1.2883	2.5403	0.0000
C	2.5257	-1.1829	0.0000	C	-3.4356	-0.1242	0.0000	H	-1.2897	2.5395	0.0000
C	3.4357	-0.1222	0.0000	C	-2.5250	-1.1843	0.0000	H	-3.7318	2.0090	0.0000
C	2.9980	1.1974	0.0000	H	0.0007	-2.4855	0.8885	H	-4.5093	-0.3392	0.0000
C	1.6352	1.5020	0.0000	H	0.0007	-2.4855	-0.8885	H	-2.8739	-2.2214	0.0000
C	-1.1746	-0.8903	0.0000	H	2.8752	-2.2197	0.0000				

Table 3.14: Table of thermodynamic data as a function of temperature for Fluorene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-26.717	189.836	189.836	∞
100	60.744	273.779	497.492	-22.371	197.252	221.475	-115.684
200	111.175	330.240	399.935	-13.939	187.976	249.353	-65.123
250	142.404	358.357	388.796	-7.610	183.477	265.219	-55.413
298.15	173.708	386.113	386.113	0.000	179.400	281.340	-49.289
300	174.907	387.191	386.116	0.322	179.249	281.972	-49.095
350	206.654	416.557	388.363	9.868	175.427	299.402	-44.682
400	236.336	446.117	393.734	20.953	172.051	317.344	-41.440
450	263.348	475.540	401.192	33.457	169.086	335.686	-38.965
500	287.575	504.565	410.082	47.241	166.486	354.349	-37.018
600	328.409	560.749	430.550	78.119	162.205	392.344	-34.156
700	360.988	613.911	452.985	112.648	158.995	430.972	-32.159
800	387.390	663.897	476.258	150.111	156.720	469.985	-30.686
900	409.134	710.820	499.741	189.971	155.255	509.233	-29.554
1000	427.270	754.893	523.075	231.818	154.483	548.611	-28.656
1100	442.539	796.353	546.053	275.330	154.278	588.042	-27.923
1200	455.489	835.429	568.555	320.249	154.544	627.462	-27.312
1300	466.538	872.336	590.517	366.365	155.168	666.851	-26.794
1400	476.014	907.266	611.905	413.504	156.067	706.182	-26.347
1500	484.182	940.393	632.710	461.524	157.185	745.442	-25.958
1600	491.255	971.872	652.932	510.304	158.445	784.618	-25.615
1700	497.408	1001.843	672.582	559.744	159.799	823.698	-25.309
1800	502.785	1030.430	691.674	609.760	161.204	862.731	-25.035
1900	507.503	1057.743	710.228	660.279	162.636	901.658	-24.788
2000	511.660	1083.883	728.262	711.242	164.062	940.523	-24.563
2100	515.337	1108.937	745.797	762.595	165.438	979.310	-24.358
2200	518.603	1132.988	762.853	814.296	166.763	1018.036	-24.171
2300	521.515	1156.106	779.452	866.304	168.027	1056.699	-23.998
2400	524.119	1178.357	795.612	918.588	169.196	1095.288	-23.838
2500	526.456	1199.801	811.354	971.119	170.272	1133.887	-23.691
2600	528.560	1220.491	826.694	1023.872	171.235	1172.386	-23.553
2700	530.460	1240.475	841.651	1076.824	172.085	1210.883	-23.425
2800	532.182	1259.798	856.242	1129.958	172.810	1249.367	-23.307
2900	533.746	1278.501	870.482	1183.255	173.391	1287.798	-23.195
3000	535.170	1296.620	884.386	1236.702	173.851	1326.223	-23.091
3100	536.470	1314.190	897.969	1290.285	174.150	1364.600	-22.993
3200	537.660	1331.241	911.243	1343.993	174.308	1403.005	-22.901
3300	538.752	1347.803	924.223	1397.814	174.313	1441.425	-22.815
3400	539.756	1363.901	936.919	1451.740	174.154	1479.808	-22.734
3500	540.681	1379.561	949.343	1505.763	173.831	1518.188	-22.657
3600	541.535	1394.805	961.506	1559.874	173.353	1556.619	-22.585
3700	542.325	1409.653	973.419	1614.067	172.706	1595.079	-22.518
3800	543.057	1424.126	985.090	1668.337	171.875	1633.523	-22.454
3900	543.737	1438.241	996.529	1722.677	170.881	1671.973	-22.393
4000	544.369	1452.015	1007.744	1777.083	169.715	1710.515	-22.337
4100	544.957	1465.464	1018.745	1831.549	168.358	1749.051	-22.283
4200	545.506	1478.603	1029.538	1886.073	166.826	1787.618	-22.232
4300	546.020	1491.445	1040.131	1940.649	165.108	1826.181	-22.183
4400	546.500	1504.003	1050.532	1995.276	163.213	1864.832	-22.138
4500	546.949	1516.290	1060.746	2049.948	161.143	1903.557	-22.095
4600	547.371	1528.316	1070.780	2104.665	158.877	1942.329	-22.055
4700	547.768	1540.092	1080.641	2159.422	156.418	1981.098	-22.017
4800	548.140	1551.628	1090.333	2214.217	153.792	2019.973	-21.981
4900	548.491	1562.934	1099.863	2269.049	150.962	2058.839	-21.947
5000	548.822	1574.019	1109.236	2323.915	147.974	2097.860	-21.916

3.15. 1*H*-Benz[*f*]indene



Other names: 1*H*- β -Naphthindene

Formula: C₁₃H₁₀

Mass: 166.219 g/mol

CAS Number: 268-40-6

Point Group: C_s

Length: 11.48 Å

Width: 7.434 Å

Breadth: 4.174 Å

L/B Ratio: 1.544

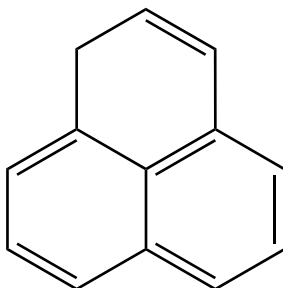
Cartesian coordinates:

C	-2.8615	1.1297	-0.0000	C	0.9549	-0.6893	-0.0000	H	-3.0805	-1.8497	-0.8884
C	-3.6617	0.0439	0.0000	C	2.2040	-1.3647	-0.0000	H	-0.2420	-2.5200	0.0000
C	-2.8586	-1.2305	0.0000	C	3.3760	-0.6565	0.0000	H	-0.3141	2.5200	0.0000
C	-1.4613	0.7000	-0.0000	C	3.3571	0.7564	0.0000	H	2.2125	-2.4605	-0.0000
C	-1.4418	-0.7361	0.0000	C	2.1665	1.4327	0.0000	H	4.3396	-1.1763	0.0000
C	-0.2675	-1.4252	-0.0000	H	-3.1623	2.1762	-0.0000	H	4.3063	1.3019	0.0000
C	-0.3053	1.4250	0.0000	H	-4.7502	0.0314	0.0000	H	2.1451	2.5283	0.0000
C	0.9358	0.7236	0.0000	H	-3.0805	-1.8497	0.8884				

Table 3.15: Table of thermodynamic data as a function of temperature for 1*H*-Benz[*f*]indene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-26.840	230.632	230.632	∞
100	60.182	278.827	504.227	-22.540	248.315	272.034	-142.093
200	112.186	335.468	405.831	-14.072	239.075	299.406	-78.195
250	143.798	363.856	394.585	-7.682	234.637	315.003	-65.815
298.15	175.302	391.877	391.877	0.000	230.632	330.853	-57.963
300	176.506	392.965	391.880	0.325	230.485	331.475	-57.714
350	208.303	422.583	394.146	9.953	226.744	348.610	-52.026
400	237.931	452.360	399.562	21.119	223.449	366.245	-47.826
450	264.836	481.966	407.076	33.700	220.561	384.270	-44.604
500	288.932	511.140	416.029	47.556	218.033	402.608	-42.059
600	329.508	567.548	436.621	78.556	213.874	439.934	-38.299
700	361.869	620.863	459.172	113.184	210.763	477.873	-35.659
800	388.101	670.955	482.547	150.726	208.568	516.186	-33.703
900	409.713	717.954	506.120	190.651	207.167	554.723	-32.195
1000	427.748	762.083	529.533	232.550	206.447	593.385	-30.995
1100	442.939	803.584	552.579	276.106	206.286	632.096	-30.015
1200	455.828	842.693	575.141	321.061	206.589	670.791	-29.198
1300	466.827	879.624	597.156	367.208	207.244	709.452	-28.506
1400	476.264	914.574	618.592	414.375	208.170	748.054	-27.910
1500	484.400	947.717	639.438	462.418	209.311	786.582	-27.391
1600	491.446	979.210	659.698	511.219	210.592	825.024	-26.934
1700	497.577	1009.192	679.382	560.677	211.964	863.371	-26.528
1800	502.935	1037.787	698.505	610.708	213.384	901.668	-26.165
1900	507.637	1065.108	717.086	661.242	214.831	939.859	-25.838
2000	511.781	1091.254	735.146	712.217	216.269	977.987	-25.542
2100	515.447	1116.315	752.704	763.582	217.657	1016.036	-25.272
2200	518.703	1140.370	769.782	815.293	218.992	1054.024	-25.025
2300	521.606	1163.493	786.401	867.311	220.266	1091.949	-24.798
2400	524.202	1185.748	802.579	919.604	221.444	1129.799	-24.589
2500	526.533	1207.195	818.338	972.143	222.528	1167.658	-24.396
2600	528.631	1227.887	833.694	1024.903	223.498	1205.418	-24.217
2700	530.526	1247.874	848.666	1077.862	224.355	1243.175	-24.050
2800	532.243	1267.200	863.270	1131.002	225.086	1280.919	-23.895
2900	533.802	1285.905	877.523	1184.306	225.674	1318.610	-23.750
3000	535.223	1304.026	891.440	1237.758	226.139	1356.294	-23.615
3100	536.520	1321.597	905.034	1291.346	226.443	1393.931	-23.487
3200	537.707	1338.650	918.319	1345.058	226.605	1431.595	-23.368
3300	538.796	1355.213	931.308	1398.884	226.615	1469.274	-23.256
3400	539.797	1371.312	944.014	1452.814	226.461	1506.916	-23.150
3500	540.720	1386.973	956.447	1506.841	226.141	1544.555	-23.051
3600	541.572	1402.218	968.619	1560.956	225.667	1582.244	-22.957
3700	542.360	1417.067	980.540	1615.153	225.024	1619.964	-22.869
3800	543.090	1431.541	992.218	1669.426	224.196	1657.666	-22.786
3900	543.768	1445.657	1003.665	1723.769	223.206	1695.374	-22.707
4000	544.398	1459.432	1014.887	1778.178	222.042	1733.174	-22.632
4100	544.986	1472.882	1025.895	1832.648	220.689	1770.969	-22.562
4200	545.533	1486.021	1036.694	1887.174	219.159	1808.795	-22.495
4300	546.045	1498.864	1047.294	1941.753	217.444	1846.615	-22.431
4400	546.524	1511.423	1057.700	1996.382	215.551	1884.524	-22.372
4500	546.973	1523.710	1067.920	2051.057	213.484	1922.508	-22.315
4600	547.394	1535.736	1077.959	2105.775	211.220	1960.538	-22.262
4700	547.789	1547.513	1087.825	2160.535	208.763	1998.565	-22.211
4800	548.161	1559.050	1097.522	2215.332	206.140	2036.697	-22.163
4900	548.511	1570.356	1107.057	2270.166	203.311	2074.821	-22.117
5000	548.841	1581.441	1116.434	2325.034	200.325	2113.100	-22.075

3.16. Phenalene



Other names: 1*H*-Benzonaphthene
Perinaphthene
H-Phenalene
Phenalin

Formula: C₁₃H₁₀
Mass: 166.219 g/mol
CAS Number: 203-80-5
Point Group: C_s

Length: 9.568 Å
Width: 9.134 Å
Breadth: 4.169 Å
L/B Ratio: 1.048

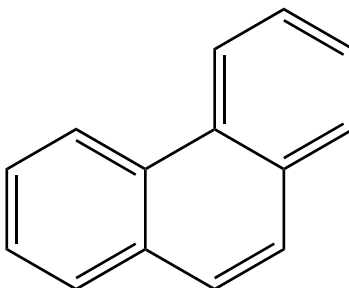
Cartesian coordinates:

C	-1.5997	-1.8110	0.0000	C	0.3350	1.3779	0.0000	H	3.2218	-1.2458	0.0000
C	-0.5497	-2.7547	0.0000	C	-0.7567	2.3390	0.0000	H	3.7297	1.1869	0.0000
C	0.7562	-2.3439	0.0000	C	-2.0352	1.9456	0.0000	H	1.8981	2.8543	0.0000
C	1.0682	-0.9583	0.0000	C	-2.4526	0.5216	0.0000	H	-0.4888	3.4021	0.0000
C	2.4144	-0.5051	0.0000	C	-1.3303	-0.4623	0.0000	H	-2.8473	2.6816	0.0000
C	2.6925	0.8360	0.0000	H	-2.6363	-2.1657	0.0000	H	-3.0968	0.3394	0.8856
C	1.6499	1.7870	0.0000	H	-0.7965	-3.8215	0.0000	H	-3.0968	0.3394	-0.8856
C	0.0213	-0.0138	0.0000	H	1.5751	-3.0717	0.0000				

Table 3.16: Table of thermodynamic data as a function of temperature for Phenalene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-26.482	215.746	215.746	∞
100	58.925	277.925	500.125	-22.220	233.749	257.557	-134.531
200	110.703	333.494	403.032	-13.908	224.353	285.080	-74.454
250	142.141	361.537	391.916	-7.595	219.838	300.784	-62.844
298.15	173.308	389.238	389.238	0.000	215.746	316.753	-55.493
300	174.499	390.314	389.241	0.322	215.594	317.380	-55.260
350	205.988	419.598	391.482	9.840	211.745	334.656	-49.944
400	235.432	449.053	396.838	20.886	208.330	352.448	-46.024
450	262.275	478.359	404.270	33.340	205.315	370.646	-43.023
500	286.408	507.265	413.129	47.068	202.659	389.172	-40.656
600	327.224	563.232	433.520	77.827	198.258	426.908	-37.165
700	359.910	616.218	455.872	112.242	194.935	465.296	-34.720
800	386.464	666.070	479.064	149.605	192.560	504.086	-32.913
900	408.359	712.893	502.471	189.380	191.010	543.121	-31.521
1000	426.631	756.892	525.735	231.157	190.167	582.296	-30.415
1100	442.014	798.296	548.650	274.610	189.904	621.530	-29.513
1200	455.058	837.331	571.096	319.482	190.122	660.758	-28.761
1300	466.182	874.206	593.008	365.558	190.707	699.958	-28.124
1400	475.718	909.112	614.351	412.665	191.574	739.104	-27.576
1500	483.935	942.220	635.115	460.658	192.664	778.180	-27.098
1600	491.047	973.685	655.300	509.415	193.902	817.174	-26.677
1700	497.232	1003.644	674.917	558.836	195.237	856.074	-26.303
1800	502.634	1032.222	693.980	608.836	196.625	894.927	-25.970
1900	507.373	1059.527	712.506	659.341	198.044	933.675	-25.668
2000	511.548	1085.661	730.515	710.291	199.457	972.362	-25.395
2100	515.240	1110.710	748.027	761.634	200.823	1010.971	-25.146
2200	518.518	1134.756	765.063	813.326	202.138	1049.520	-24.918
2300	521.439	1157.871	781.642	865.326	203.395	1088.007	-24.709
2400	524.052	1180.119	797.785	917.603	204.557	1126.420	-24.515
2500	526.396	1201.561	813.510	970.127	205.626	1164.842	-24.338
2600	528.506	1222.248	828.835	1022.874	206.583	1203.165	-24.171
2700	530.412	1242.230	843.778	1075.822	207.429	1241.487	-24.018
2800	532.138	1261.552	858.355	1128.951	208.149	1279.795	-23.874
2900	533.706	1280.253	872.583	1182.244	208.726	1318.051	-23.740
3000	535.134	1298.371	886.475	1235.687	209.182	1356.301	-23.615
3100	536.437	1315.940	900.047	1289.267	209.478	1394.503	-23.497
3200	537.630	1332.990	913.311	1342.971	209.632	1432.733	-23.386
3300	538.725	1349.551	926.281	1396.790	209.634	1470.978	-23.283
3400	539.731	1365.648	938.968	1450.713	209.473	1509.186	-23.185
3500	540.657	1381.307	951.384	1504.733	209.147	1547.391	-23.093
3600	541.513	1396.550	963.539	1558.842	208.667	1585.648	-23.007
3700	542.305	1411.398	975.443	1613.034	208.018	1623.934	-22.925
3800	543.038	1425.870	987.107	1667.301	207.185	1662.204	-22.848
3900	543.719	1439.985	998.539	1721.640	206.189	1700.478	-22.775
4000	544.352	1453.759	1009.748	1776.044	205.021	1738.846	-22.707
4100	544.942	1467.208	1020.742	1830.509	203.663	1777.208	-22.641
4200	545.492	1480.346	1031.529	1885.031	202.129	1815.601	-22.580
4300	546.006	1493.188	1042.117	1939.606	200.410	1853.989	-22.521
4400	546.487	1505.746	1052.512	1994.231	198.513	1892.466	-22.466
4500	546.937	1518.032	1062.720	2048.902	196.443	1931.017	-22.414
4600	547.360	1530.058	1072.750	2103.617	194.175	1969.615	-22.365
4700	547.757	1541.834	1082.605	2158.373	191.715	2008.210	-22.318
4800	548.130	1553.370	1092.293	2213.168	189.088	2046.910	-22.274
4900	548.481	1564.676	1101.819	2267.998	186.257	2085.602	-22.232
5000	548.813	1575.760	1111.187	2322.863	183.268	2124.449	-22.194

3.17. Phenanthrene



Other names: Phenanthrin
Formula: $C_{14}H_{10}$
Mass: 178.229 g/mol
CAS Number: 85-01-8
Point Group: C_{2v}

Length: 11.64 Å
Width: 7.956 Å
Breadth: 3.883 Å
L/B Ratio: 1.462

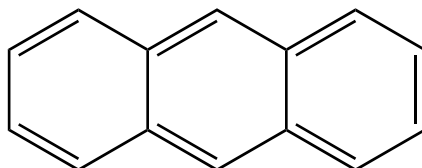
Cartesian coordinates:

C	2.8230	-0.8727	0.0000	C	-1.4146	-0.8605	0.0000	H	3.4073	2.4740	0.0000
C	3.5237	0.3120	0.0000	C	-0.7224	0.3632	0.0000	H	0.9101	2.5149	0.0000
C	2.8386	1.5385	0.0000	C	-1.4571	1.5683	0.0000	H	-1.2473	-3.0341	0.0000
C	1.4629	1.5629	0.0000	C	-2.8329	1.5490	0.0000	H	1.2361	-3.0387	0.0000
C	1.4114	-0.8657	0.0000	C	-3.5225	0.3250	0.0000	H	-0.9009	2.5183	0.0000
C	0.7238	0.3605	0.0000	C	-2.8262	-0.8623	0.0000	H	-3.3982	2.4866	0.0000
C	-0.6809	-2.0957	0.0000	H	3.3527	-1.8321	0.0000	H	-4.6173	0.3238	0.0000
C	0.6732	-2.0982	0.0000	H	4.6185	0.3067	0.0000	H	-3.3594	-1.8197	0.0000

Table 3.17: Table of thermodynamic data as a function of temperature for Phenanthrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-27.943	212.555	212.555	∞
100	62.305	278.108	513.246	-23.514	219.100	242.986	-126.920
200	117.051	336.866	410.490	-14.725	209.855	270.524	-70.652
250	150.497	366.538	398.718	-8.045	205.411	286.205	-59.798
298.15	183.654	395.882	395.882	0.000	201.400	302.138	-52.932
300	184.919	397.022	395.885	0.341	201.252	302.763	-52.715
350	218.314	428.058	398.260	10.429	197.501	319.986	-47.754
400	249.422	459.270	403.936	22.134	194.193	337.710	-44.099
450	277.672	490.308	411.811	35.324	191.286	355.826	-41.302
500	302.974	520.899	421.195	49.852	188.732	374.259	-39.098
600	345.545	580.051	442.784	82.361	184.504	411.781	-35.848
700	379.426	635.958	466.427	118.672	181.303	449.930	-33.574
800	406.817	688.473	490.936	158.030	179.002	488.467	-31.893
900	429.328	737.731	515.650	199.873	177.485	527.241	-30.600
1000	448.075	783.964	540.194	243.771	176.641	566.154	-29.572
1100	463.842	827.431	564.350	289.389	176.348	605.129	-28.735
1200	477.205	868.379	587.997	336.459	176.514	644.100	-28.036
1300	488.601	907.038	611.065	384.764	177.028	683.048	-27.445
1400	498.373	943.614	633.524	434.125	177.809	721.949	-26.936
1500	506.796	978.293	655.363	484.394	178.802	760.786	-26.492
1600	514.089	1011.239	676.584	535.447	179.930	799.548	-26.102
1700	520.434	1042.600	697.200	587.180	181.145	838.223	-25.755
1800	525.978	1072.508	717.226	639.507	182.404	876.859	-25.445
1900	530.844	1101.079	736.682	692.353	183.684	915.397	-25.166
2000	535.131	1128.419	755.591	745.656	184.951	953.882	-24.912
2100	538.925	1154.622	773.973	799.363	186.162	992.296	-24.682
2200	542.294	1179.772	791.850	853.427	187.313	1030.657	-24.470
2300	545.298	1203.945	809.245	907.810	188.399	1068.965	-24.276
2400	547.985	1227.211	826.179	962.476	189.380	1107.203	-24.097
2500	550.397	1249.630	842.671	1017.398	190.262	1145.463	-23.933
2600	552.568	1271.260	858.742	1072.548	191.022	1183.628	-23.779
2700	554.530	1292.152	874.410	1127.904	191.662	1221.802	-23.637
2800	556.307	1312.351	889.692	1183.448	192.169	1259.970	-23.505
2900	557.921	1331.902	904.605	1239.160	192.523	1298.091	-23.381
3000	559.391	1350.841	919.165	1295.027	192.749	1336.217	-23.265
3100	560.734	1369.206	933.388	1351.034	192.804	1374.299	-23.156
3200	561.963	1387.028	947.287	1407.170	192.710	1412.419	-23.055
3300	563.090	1404.338	960.876	1463.423	192.455	1450.564	-22.960
3400	564.127	1421.164	974.168	1519.785	192.027	1488.676	-22.870
3500	565.082	1437.530	987.174	1576.246	191.425	1526.794	-22.786
3600	565.964	1453.462	999.906	1632.799	190.661	1564.973	-22.707
3700	566.780	1468.980	1012.375	1689.437	189.719	1603.190	-22.633
3800	567.536	1484.105	1024.591	1746.153	188.582	1641.399	-22.562
3900	568.238	1498.856	1036.563	1802.942	187.274	1679.617	-22.495
4000	568.890	1513.251	1048.301	1859.799	185.785	1717.941	-22.434
4100	569.498	1527.306	1059.813	1916.719	184.096	1756.266	-22.375
4200	570.066	1541.036	1071.108	1973.697	182.221	1794.630	-22.319
4300	570.596	1554.456	1082.194	2030.730	180.152	1832.993	-22.266
4400	571.091	1567.580	1093.076	2087.815	177.896	1871.457	-22.217
4500	571.556	1580.419	1103.764	2144.948	175.458	1910.004	-22.170
4600	571.992	1592.986	1114.263	2202.125	172.811	1948.608	-22.127
4700	572.401	1605.292	1124.580	2259.345	169.963	1987.213	-22.085
4800	572.786	1617.347	1134.721	2316.605	166.940	2025.936	-22.046
4900	573.149	1629.161	1144.692	2373.902	163.701	2064.654	-22.009
5000	573.491	1640.744	1154.497	2431.234	160.296	2103.541	-21.975

3.18. Anthracene



Other names: Anthracin
Paranaphthalene

Formula: C₁₄H₁₀

Mass: 178.229 g/mol

CAS Number: 120-12-7

Point Group: D_{2h}

Length: 11.60 Å

Width: 7.408 Å

Breadth: 3.882 Å

L/B Ratio: 1.566

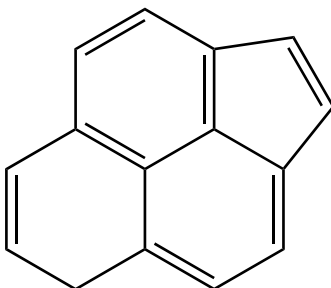
Cartesian coordinates:

C	-3.6379	0.7140	0.0000	C	1.2129	0.7103	0.0000	H	-2.4580	-2.4988	0.0000
C	-3.6385	-0.7112	0.0000	C	1.2124	-0.7112	0.0000	H	-2.4561	2.5007	0.0000
C	-2.4676	-1.4030	0.0000	C	2.4666	-1.4048	0.0000	H	-0.0009	-2.5011	0.0000
C	-2.4666	1.4048	0.0000	C	3.6379	-0.7139	0.0000	H	0.0009	2.5011	0.0000
C	-1.2124	0.7112	0.0000	C	3.6384	0.7113	0.0000	H	2.4562	-2.5007	0.0000
C	-1.2129	-0.7103	0.0000	C	2.4676	1.4030	0.0000	H	4.5986	-1.2391	0.0000
C	-0.0005	-1.4041	0.0000	H	-4.5986	1.2392	0.0000	H	4.5995	1.2358	0.0000
C	0.0005	1.4041	0.0000	H	-4.5995	-1.2357	0.0000	H	2.4580	2.4988	0.0000

Table 3.18: Table of thermodynamic data as a function of temperature for Anthracene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-27.941	232.473	232.473	∞
100	61.835	271.550	507.149	-23.560	248.554	273.095	-142.647
200	117.379	330.273	404.130	-14.771	239.309	301.296	-78.689
250	150.994	360.039	392.321	-8.070	234.886	317.305	-66.296
298.15	184.194	389.475	389.475	0.000	230.900	333.549	-58.435
300	185.459	390.618	389.479	0.342	230.753	334.185	-58.186
350	218.815	421.736	391.860	10.457	227.029	351.726	-52.491
400	249.848	453.010	397.549	22.184	223.743	369.764	-48.285
450	278.018	484.094	405.442	35.393	220.855	388.193	-45.059
500	303.250	514.717	414.843	49.937	218.317	406.935	-42.511
600	345.725	573.910	436.463	82.468	214.111	445.073	-38.746
700	379.558	629.840	460.134	118.794	210.925	483.835	-36.103
800	406.929	682.372	484.666	158.165	208.637	522.983	-34.147
900	429.435	731.642	509.400	200.018	207.130	562.367	-32.638
1000	448.181	777.887	533.960	243.927	206.297	601.888	-31.439
1100	463.948	821.364	558.132	289.556	206.015	641.469	-30.460
1200	477.311	862.321	581.791	336.637	206.192	681.047	-29.645
1300	488.706	900.988	604.871	384.952	206.716	720.601	-28.953
1400	498.476	937.572	627.341	434.324	207.508	760.106	-28.359
1500	506.894	972.257	649.189	484.602	208.510	799.547	-27.842
1600	514.184	1005.210	670.419	535.665	209.648	838.912	-27.387
1700	520.525	1036.577	691.043	587.408	210.873	878.189	-26.983
1800	526.065	1066.489	711.077	639.743	212.140	917.428	-26.623
1900	530.926	1095.065	730.540	692.598	213.429	956.568	-26.297
2000	535.210	1122.410	749.455	745.909	214.704	995.653	-26.003
2100	538.999	1148.616	767.843	799.623	215.922	1034.668	-25.735
2200	542.365	1173.769	785.726	853.695	217.081	1073.630	-25.491
2300	545.364	1197.946	803.127	908.084	218.173	1112.537	-25.266
2400	548.048	1221.214	820.065	962.757	219.161	1151.376	-25.059
2500	550.456	1243.636	836.563	1017.684	220.048	1190.235	-24.868
2600	552.625	1265.269	852.638	1072.840	220.814	1228.999	-24.690
2700	554.583	1286.162	868.309	1128.202	221.460	1267.772	-24.526
2800	556.357	1306.364	883.595	1183.751	221.972	1306.539	-24.373
2900	557.969	1325.915	898.513	1239.468	222.331	1345.259	-24.230
3000	559.437	1344.857	913.077	1295.340	222.562	1383.983	-24.097
3100	560.777	1363.223	927.303	1351.351	222.621	1422.664	-23.971
3200	562.004	1381.046	941.205	1407.491	222.531	1461.382	-23.854
3300	563.129	1398.357	954.797	1463.749	222.281	1500.125	-23.745
3400	564.164	1415.184	968.092	1520.114	221.856	1538.836	-23.641
3500	565.117	1431.552	981.101	1576.579	221.258	1577.551	-23.543
3600	565.997	1447.484	993.835	1633.135	220.497	1616.328	-23.452
3700	566.812	1463.003	1006.307	1689.776	219.558	1655.143	-23.366
3800	567.566	1478.129	1018.525	1746.496	218.425	1693.949	-23.284
3900	568.267	1492.881	1030.500	1803.288	217.120	1732.765	-23.207
4000	568.918	1507.277	1042.240	1860.147	215.633	1771.687	-23.135
4100	569.525	1521.332	1053.754	1917.070	213.947	1810.609	-23.067
4200	570.091	1535.063	1065.051	1974.051	212.075	1849.569	-23.002
4300	570.620	1548.484	1076.138	2031.087	210.009	1888.530	-22.941
4400	571.115	1561.608	1087.023	2088.174	207.755	1927.591	-22.883
4500	571.579	1574.448	1097.713	2145.309	205.319	1966.736	-22.829
4600	572.014	1587.015	1108.214	2202.489	202.675	2005.937	-22.778
4700	572.422	1599.322	1118.532	2259.711	199.829	2045.139	-22.729
4800	572.806	1611.377	1128.675	2316.972	196.807	2084.459	-22.683
4900	573.168	1623.192	1138.647	2374.271	193.570	2123.774	-22.639
5000	573.509	1634.775	1148.454	2431.605	190.167	2163.258	-22.599

3.19. 5H-Benz[fg]acenaphthylene



Formula: C₁₅H₁₀
Mass: 190.240 g/mol
CAS Number: 194-27-4
Point Group: C_s

Length: 10.74 Å
Width: 9.175 Å
Breadth: 4.169 Å
L/B Ratio: 1.170

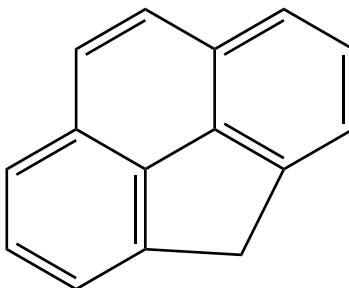
Cartesian coordinates:

C	-1.1410	-1.2736	0.0000	C	1.6679	1.1965	0.0000	H	-0.9148	3.3897	0.0000
C	-0.3600	-2.4128	0.0000	C	-2.6311	-1.2964	-0.0000	H	-0.8468	-3.3946	0.0000
C	1.0638	-2.3721	0.0000	C	-3.2738	0.0485	-0.0000	H	1.6275	-3.3101	0.0000
C	1.6927	-1.1547	0.0000	C	-2.6163	1.2182	0.0000	H	-3.1524	2.1739	0.0000
C	0.8745	0.0123	0.0000	C	3.0755	-0.6468	0.0000	H	-4.3704	0.0377	-0.0000
C	-0.5050	-0.0022	0.0000	C	3.0609	0.7179	-0.0000	H	-2.9900	-1.8611	0.8857
C	-1.1639	1.2605	0.0000	H	3.9506	-1.2932	-0.0000	H	-2.9900	-1.8611	-0.8857
C	-0.4072	2.4183	0.0000	H	3.9221	1.3828	-0.0000				
C	1.0158	2.4028	0.0000	H	1.5638	3.3501	-0.0000				

Table 3.19: Table of thermodynamic data as a function of temperature for 5*H*-Benz[*fg*]acenaphthylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-28.804	330.939	330.939	∞
100	62.401	283.855	528.278	-24.442	348.702	372.108	-194.365
200	121.889	344.062	421.145	-15.417	339.367	399.213	-104.262
250	157.632	375.065	408.811	-8.436	334.928	414.689	-86.643
298.15	192.733	405.835	405.835	0.000	330.939	430.421	-75.406
300	194.068	407.032	405.839	0.358	330.792	431.038	-75.049
350	229.243	439.615	408.332	10.949	327.073	448.047	-66.866
400	261.938	472.392	414.291	23.240	323.799	465.553	-60.794
450	291.606	504.987	422.561	37.092	320.926	483.447	-56.116
500	318.174	537.113	432.415	52.349	318.403	501.654	-52.406
600	362.871	599.232	455.085	86.488	314.227	538.716	-46.898
700	398.414	657.940	479.913	124.619	311.073	576.397	-43.010
800	427.090	713.078	505.650	165.943	308.817	614.458	-40.119
900	450.590	764.783	531.601	209.865	307.344	652.752	-37.884
1000	470.094	813.298	557.370	255.928	306.542	691.179	-36.103
1100	486.443	858.892	582.730	303.779	306.288	729.664	-34.648
1200	500.253	901.827	607.550	353.132	306.486	768.142	-33.436
1300	511.996	942.345	631.760	403.760	307.024	806.595	-32.409
1400	522.039	980.665	655.325	455.475	307.819	845.000	-31.527
1500	530.675	1016.983	678.236	508.121	308.815	883.340	-30.760
1600	538.137	1051.476	700.495	561.571	309.935	921.605	-30.087
1700	544.618	1084.300	722.114	615.716	311.130	959.783	-29.490
1800	550.272	1115.593	743.111	670.467	312.356	997.926	-28.958
1900	555.227	1145.480	763.508	725.747	313.591	1035.971	-28.480
2000	559.588	1174.073	783.327	781.493	314.802	1073.966	-28.049
2100	563.443	1201.470	802.590	837.648	315.942	1111.894	-27.656
2200	566.863	1227.762	821.323	894.167	317.011	1149.772	-27.298
2300	569.909	1253.029	839.547	951.008	318.002	1187.600	-26.971
2400	572.632	1277.343	857.285	1008.138	318.877	1225.363	-26.669
2500	575.075	1300.769	874.559	1065.525	319.639	1263.154	-26.392
2600	577.273	1323.367	891.389	1123.145	320.269	1300.852	-26.134
2700	579.258	1345.192	907.794	1180.973	320.767	1338.568	-25.896
2800	581.055	1366.291	923.795	1238.990	321.119	1376.282	-25.674
2900	582.686	1386.710	939.407	1297.178	321.307	1413.955	-25.468
3000	584.171	1406.489	954.648	1355.522	321.356	1451.639	-25.275
3100	585.527	1425.667	969.535	1414.008	321.222	1489.282	-25.094
3200	586.768	1444.276	984.081	1472.624	320.928	1526.972	-24.925
3300	587.906	1462.350	998.302	1531.358	320.462	1564.696	-24.767
3400	588.952	1479.916	1012.210	1590.202	319.811	1602.389	-24.617
3500	589.915	1497.002	1025.818	1649.146	318.975	1640.094	-24.477
3600	590.805	1513.634	1039.138	1708.183	317.967	1677.872	-24.345
3700	591.627	1529.832	1052.182	1767.305	316.769	1715.693	-24.221
3800	592.390	1545.620	1064.961	1826.506	315.365	1753.512	-24.103
3900	593.097	1561.017	1077.484	1885.781	313.780	1791.345	-23.992
4000	593.755	1576.041	1089.761	1945.124	312.003	1829.297	-23.888
4100	594.368	1590.710	1101.801	2004.530	310.014	1867.254	-23.789
4200	594.939	1605.040	1113.613	2063.996	307.830	1905.257	-23.695
4300	595.473	1619.046	1125.205	2123.517	305.441	1943.265	-23.605
4400	595.972	1632.741	1136.584	2183.089	302.853	1981.382	-23.522
4500	596.440	1646.140	1147.760	2242.710	300.074	2019.593	-23.442
4600	596.879	1659.254	1158.737	2302.376	297.075	2057.870	-23.367
4700	597.291	1672.095	1169.523	2362.085	293.864	2096.151	-23.296
4800	597.679	1684.674	1180.125	2421.834	290.468	2134.562	-23.228
4900	598.044	1697.001	1190.548	2481.620	286.844	2172.970	-23.164
5000	598.388	1709.087	1200.798	2541.442	283.046	2211.562	-23.104

3.20. 4*H*-Cyclopenta[*def*]phenanthrene



Other names: Benzo[*def*]fluorene
Cyclopentaphenanthrene
4,5-Methylenephenanthrene
4,5-Phenanthrylenemethane

Formula: C₁₅H₁₀
Mass: 190.240 g/mol
CAS Number: 203-64-5
Point Group: C_{2v}

Length: 11.31 Å
Width: 8.742 Å
Breadth: 4.178 Å
L/B Ratio: 1.293

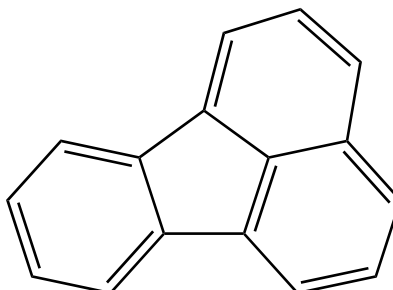
Cartesian coordinates:

C	-0.1933	2.2870	-0.0000	C	-1.3495	-1.2571	-0.0000	H	4.3979	0.8435	0.0000
C	1.0786	1.4535	-0.0000	C	-0.7086	-0.0292	-0.0000	H	2.8147	2.7403	0.0000
C	2.9216	-0.7034	0.0000	C	-1.3073	1.2520	-0.0000	H	-0.9534	-3.4001	-0.0000
C	3.3251	0.6203	0.0000	C	-2.6802	1.2863	0.0000	H	1.5104	-3.1919	-0.0000
C	2.4263	1.7178	0.0000	C	-3.3819	0.0535	0.0000	H	-3.2343	2.2293	0.0000
C	1.5414	-1.0129	-0.0000	C	-2.7621	-1.1837	0.0000	H	-4.4771	0.0933	0.0000
C	0.7034	0.0901	-0.0000	H	-0.2484	2.9394	-0.8895	H	-3.3539	-2.1046	0.0000
C	-0.4827	-2.4109	-0.0000	H	-0.2484	2.9394	0.8895				
C	0.8804	-2.2957	-0.0000	H	3.6595	-1.5120	0.0000				

Table 3.20: Table of thermodynamic data as a function of temperature for 4*H*-Cyclopenta[*def*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-28.283	255.665	255.665	∞
100	60.304	276.463	516.818	-24.036	273.834	297.979	-155.645
200	119.823	335.244	411.321	-15.215	264.294	325.904	-85.116
250	155.571	365.786	399.141	-8.339	259.751	341.832	-71.420
298.15	190.743	396.198	396.198	0.000	255.665	358.020	-62.722
300	192.082	397.382	396.202	0.354	255.514	358.655	-62.446
350	227.387	429.669	398.671	10.849	251.699	376.154	-56.137
400	260.239	462.208	404.579	23.052	248.336	394.163	-51.471
450	290.068	494.613	412.785	36.822	245.382	412.572	-47.889
500	316.785	526.584	422.571	52.006	242.786	431.302	-45.057
600	361.735	588.474	445.107	86.020	238.485	469.429	-40.867
700	397.470	647.021	469.812	124.047	235.226	508.194	-37.921
800	426.291	702.043	495.438	165.284	232.884	547.353	-35.738
900	449.902	753.661	521.293	209.132	231.336	586.754	-34.054
1000	469.494	802.108	546.977	255.131	230.471	626.298	-32.714
1100	485.915	847.648	572.262	302.925	230.160	665.905	-31.621
1200	499.786	890.540	597.015	352.229	230.309	705.509	-30.709
1300	511.579	931.022	621.166	402.813	230.803	745.093	-29.938
1400	521.665	969.313	644.678	454.488	231.558	784.631	-29.274
1500	530.338	1005.607	667.541	507.099	232.519	824.108	-28.697
1600	537.832	1040.079	689.757	560.516	233.606	863.511	-28.190
1700	544.341	1072.885	711.336	614.633	234.772	902.830	-27.740
1800	550.019	1104.163	732.298	669.357	235.972	942.115	-27.339
1900	554.996	1134.037	752.662	724.613	237.183	981.304	-26.977
2000	559.376	1162.619	772.451	780.336	238.371	1020.444	-26.651
2100	563.248	1190.006	791.687	836.471	239.491	1059.517	-26.354
2200	566.683	1216.289	810.393	892.971	240.541	1098.542	-26.082
2300	569.743	1241.548	828.594	949.795	241.515	1137.519	-25.833
2400	572.478	1265.855	846.310	1006.909	242.374	1176.429	-25.604
2500	574.931	1289.275	863.563	1064.282	243.121	1215.370	-25.393
2600	577.139	1311.868	880.373	1121.887	243.737	1254.218	-25.197
2700	579.133	1333.688	896.761	1179.702	244.222	1293.083	-25.016
2800	580.937	1354.783	912.744	1237.707	244.562	1331.948	-24.847
2900	582.576	1375.198	928.341	1295.884	244.739	1370.772	-24.690
3000	584.068	1394.973	943.568	1354.218	244.777	1409.607	-24.543
3100	585.430	1414.147	958.440	1412.694	244.633	1448.402	-24.405
3200	586.676	1432.754	972.973	1471.300	244.330	1487.245	-24.276
3300	587.819	1450.825	987.181	1530.025	243.855	1526.120	-24.156
3400	588.870	1468.389	1001.077	1588.861	243.195	1564.967	-24.042
3500	589.838	1485.473	1014.674	1647.797	242.351	1603.824	-23.935
3600	590.731	1502.102	1027.983	1706.826	241.336	1642.755	-23.835
3700	591.558	1518.299	1041.017	1765.941	240.130	1681.730	-23.741
3800	592.323	1534.085	1053.786	1825.135	238.720	1720.702	-23.652
3900	593.034	1549.480	1066.299	1884.404	237.128	1759.689	-23.568
4000	593.695	1564.503	1078.568	1943.740	235.345	1798.795	-23.489
4100	594.310	1579.170	1090.599	2003.141	233.351	1837.906	-23.415
4200	594.884	1593.499	1102.403	2062.601	231.161	1877.063	-23.344
4300	595.420	1607.503	1113.987	2122.117	228.766	1916.225	-23.277
4400	595.922	1621.197	1125.360	2181.684	226.174	1955.497	-23.214
4500	596.392	1634.594	1136.528	2241.300	223.390	1994.862	-23.155
4600	596.833	1647.707	1147.498	2300.961	220.386	2034.293	-23.100
4700	597.247	1660.547	1158.278	2360.666	217.170	2073.729	-23.046
4800	597.636	1673.126	1168.874	2420.410	213.770	2113.294	-22.997
4900	598.003	1685.452	1179.291	2480.192	210.142	2152.858	-22.949
5000	598.349	1697.537	1189.535	2540.010	206.340	2192.604	-22.906

3.21. Fluoranthene



Other names: Benzo[*jk*]fluorene
Idryl
1,2-(1,8-Naphthalenediyl)benzene
Benz[*a*]acenaphthylene
1,2-Benzoacenaphthylene

Formula: C₁₆H₁₀
Mass: 202.251 g/mol
CAS Number: 206-44-0
Point Group: C_{2v}

Length: 11.11 Å
Width: 9.199 Å
Breadth: 3.884 Å
L/B Ratio: 1.208

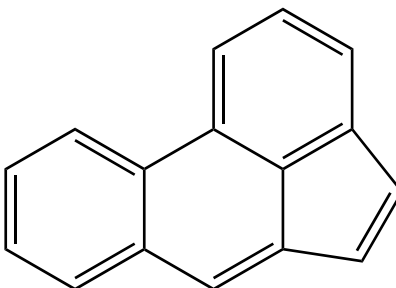
Cartesian coordinates:

C	1.1635	0.9138	0.0000	C	-0.3334	-2.4824	0.0000	H	4.3759	1.9609	0.0000
C	1.3924	-0.4999	0.0000	C	-0.8897	-0.1442	0.0000	H	2.0538	2.8773	0.0000
C	2.6774	-1.0021	0.0000	C	-0.2865	1.1516	0.0000	H	-3.7436	-1.9596	0.0000
C	3.7453	-0.0958	0.0000	C	-1.0999	2.2501	0.0000	H	-2.0660	-3.7774	0.0000
C	3.5235	1.2736	0.0000	C	-2.5088	2.0455	0.0000	H	0.3717	-3.3193	0.0000
C	2.2240	1.7961	0.0000	C	-3.0820	0.7963	0.0000	H	-0.6948	3.2667	0.0000
C	0.0918	-1.1832	0.0000	C	-2.2603	-0.3661	0.0000	H	-3.1526	2.9321	0.0000
C	-2.6731	-1.7285	0.0000	H	2.8582	-2.0816	0.0000	H	-4.1707	0.6774	0.0000
C	-1.7349	-2.7329	0.0000	H	4.7712	-0.4789	0.0000				

Table 3.21: Table of thermodynamic data as a function of temperature for Fluoranthene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-30.304	288.295	288.295	∞
100	66.973	284.681	541.957	-25.728	299.868	323.287	-168.864
200	128.115	348.544	429.373	-16.166	290.744	350.310	-91.490
250	165.253	381.079	416.444	-8.841	286.353	365.709	-76.409
298.15	201.943	413.326	413.326	0.000	282.400	381.360	-66.811
300	203.341	414.579	413.329	0.375	282.254	381.974	-66.506
350	240.184	448.718	415.941	11.472	278.570	398.892	-59.530
400	274.432	483.059	422.185	24.350	275.331	416.302	-54.362
450	305.486	517.208	430.849	38.861	272.489	434.097	-50.388
500	333.257	550.859	441.173	54.843	269.993	452.202	-47.240
600	379.868	615.907	464.921	90.592	265.849	489.052	-42.575
700	416.806	677.345	490.924	130.495	262.694	526.519	-39.289
800	446.514	735.010	517.870	173.713	260.411	564.367	-36.849
900	470.800	789.050	545.031	219.618	258.886	602.452	-34.965
1000	490.921	839.728	571.994	267.734	258.014	640.678	-33.465
1100	507.768	887.331	598.519	317.693	257.674	678.971	-32.241
1200	521.990	932.139	624.472	369.201	257.776	717.264	-31.221
1300	534.078	974.411	649.780	422.020	258.206	755.541	-30.357
1400	544.414	1014.378	674.409	475.958	258.884	793.777	-29.616
1500	553.302	1052.250	698.347	530.855	259.757	831.959	-28.971
1600	560.982	1088.210	721.599	586.578	260.745	870.073	-28.404
1700	567.653	1122.424	744.179	643.017	261.802	908.108	-27.902
1800	573.474	1155.039	766.106	700.080	262.883	946.118	-27.455
1900	578.575	1186.185	787.401	757.688	263.967	984.037	-27.053
2000	583.066	1215.978	808.091	815.775	265.020	1021.915	-26.689
2100	587.036	1244.524	828.199	874.284	265.995	1059.734	-26.359
2200	590.559	1271.916	847.749	933.167	266.891	1097.510	-26.058
2300	593.697	1298.238	866.767	992.383	267.704	1135.245	-25.782
2400	596.503	1323.566	885.276	1051.896	268.392	1172.920	-25.527
2500	599.020	1347.968	903.299	1111.674	268.960	1210.637	-25.294
2600	601.285	1371.507	920.857	1171.691	269.387	1248.263	-25.077
2700	603.330	1394.239	937.971	1231.924	269.676	1285.918	-24.877
2800	605.182	1416.215	954.661	1292.351	269.810	1323.580	-24.691
2900	606.864	1437.481	970.945	1352.955	269.772	1361.206	-24.517
3000	608.395	1458.081	986.841	1413.719	269.587	1398.853	-24.356
3100	609.793	1478.053	1002.366	1474.629	269.209	1436.464	-24.204
3200	611.072	1497.434	1017.536	1535.673	268.663	1474.132	-24.062
3300	612.246	1516.256	1032.365	1596.840	267.938	1511.844	-23.930
3400	613.324	1534.549	1046.867	1658.119	267.017	1549.530	-23.805
3500	614.318	1552.343	1061.056	1719.502	265.903	1587.235	-23.688
3600	615.235	1569.662	1074.945	1780.980	264.608	1625.024	-23.578
3700	616.083	1586.530	1088.545	1842.547	263.115	1662.865	-23.475
3800	616.869	1602.971	1101.867	1904.195	261.406	1700.711	-23.377
3900	617.599	1619.004	1114.922	1965.919	259.507	1738.576	-23.285
4000	618.278	1634.649	1127.720	2027.713	257.407	1776.573	-23.199
4100	618.909	1649.923	1140.271	2089.573	255.086	1814.581	-23.118
4200	619.499	1664.845	1152.584	2151.494	252.560	1852.643	-23.041
4300	620.050	1679.428	1164.668	2213.471	249.819	1890.715	-22.967
4400	620.565	1693.689	1176.529	2275.502	246.871	1928.908	-22.899
4500	621.047	1707.640	1188.177	2337.583	243.723	1967.204	-22.834
4600	621.500	1721.295	1199.619	2399.711	240.345	2005.576	-22.774
4700	621.925	1734.666	1210.861	2461.882	236.744	2043.956	-22.716
4800	622.325	1747.764	1221.911	2524.095	232.950	2082.478	-22.662
4900	622.702	1760.600	1232.774	2586.347	228.918	2121.001	-22.610
5000	623.057	1773.183	1243.457	2648.635	224.703	2159.720	-22.562

3.22. Acephenanthrene



Other names: Cyclopenta[*jk*]phenanthrene

Formula: C₁₆H₁₀

Mass: 202.251 g/mol

CAS Number: 201-06-9

Point Group: C_s

Length: 11.64 Å

Width: 9.023 Å

Breadth: 3.886 Å

L/B Ratio: 1.290

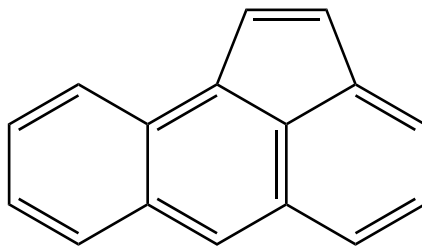
Cartesian coordinates:

C	-2.2605	2.1109	0.0000	C	2.7722	1.4744	0.0000	H	0.5944	3.0358	0.0000
C	-3.2000	1.1254	0.0000	C	-0.1506	-0.8822	0.0000	H	2.1079	-2.3560	0.0000
C	-0.9164	1.5074	0.0000	C	-1.1404	0.0826	0.0000	H	4.4440	-1.4841	0.0000
C	0.3572	1.9664	0.0000	C	-2.5340	-0.1885	0.0000	H	4.8588	0.9633	0.0000
C	1.4409	1.0060	0.0000	C	-2.9425	-1.5005	0.0000	H	2.9581	2.5548	0.0000
C	1.2102	-0.3907	0.0000	C	-1.9486	-2.5073	0.0000	H	-4.0020	-1.7729	0.0000
C	2.3052	-1.2758	0.0000	C	-0.5953	-2.2248	0.0000	H	-2.2737	-3.5535	0.0000
C	3.5952	-0.7925	0.0000	H	-2.4328	3.1853	0.0000	H	0.1489	-3.0312	0.0000
C	3.8292	0.5909	0.0000	H	-4.2814	1.2466	0.0000				

Table 3.22: Table of thermodynamic data as a function of temperature for Acephenanthrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-30.397	322.265	322.265	∞
100	66.406	290.337	548.731	-25.839	339.622	362.475	-189.334
200	128.787	354.218	435.557	-16.268	330.508	388.938	-101.578
250	166.323	386.949	422.544	-8.899	326.161	404.049	-84.420
298.15	203.244	419.406	419.406	0.000	322.265	419.413	-73.478
300	204.648	420.667	419.410	0.377	322.122	420.015	-73.130
350	241.597	455.017	422.038	11.543	318.506	436.624	-65.161
400	275.858	489.549	428.319	24.492	315.338	453.714	-59.248
450	306.867	523.863	437.032	39.074	312.567	471.180	-54.692
500	334.561	557.657	447.410	55.123	310.139	488.949	-51.079
600	380.975	622.925	471.271	90.992	306.115	525.107	-45.714
700	417.711	684.518	497.381	130.996	303.060	561.864	-41.926
800	447.242	742.292	524.424	174.295	300.858	598.989	-39.109
900	471.379	796.409	551.671	220.265	299.398	636.342	-36.932
1000	491.382	847.141	578.708	268.433	298.579	673.829	-35.197
1100	508.134	894.784	605.299	318.433	298.280	711.378	-33.780
1200	522.282	939.621	631.309	369.974	298.414	748.924	-32.599
1300	534.313	981.913	656.668	422.819	298.871	786.452	-31.599
1400	544.604	1021.897	681.341	476.778	299.570	823.937	-30.741
1500	553.456	1059.780	705.318	531.692	300.460	861.367	-29.995
1600	561.109	1095.749	728.606	587.430	301.462	898.727	-29.340
1700	567.757	1129.970	751.217	643.881	302.531	936.008	-28.759
1800	573.560	1162.590	773.172	700.953	303.621	973.264	-28.243
1900	578.648	1193.741	794.494	758.569	304.713	1010.427	-27.778
2000	583.127	1223.538	815.206	816.662	305.773	1047.550	-27.359
2100	587.088	1252.086	835.335	875.177	306.753	1084.612	-26.978
2200	590.603	1279.480	854.905	934.065	307.654	1121.632	-26.630
2300	593.735	1305.804	873.941	993.285	308.471	1158.611	-26.312
2400	596.535	1331.133	892.466	1052.801	309.162	1195.529	-26.019
2500	599.048	1355.537	910.504	1112.582	309.734	1232.489	-25.751
2600	601.309	1379.077	928.076	1172.602	310.164	1269.358	-25.501
2700	603.351	1401.810	945.203	1232.837	310.454	1306.256	-25.271
2800	605.201	1423.786	961.905	1293.266	310.590	1343.161	-25.056
2900	606.880	1445.053	978.201	1353.871	310.554	1380.030	-24.857
3000	608.410	1465.653	994.108	1414.637	310.371	1416.919	-24.670
3100	609.806	1485.626	1009.643	1475.549	309.994	1453.773	-24.495
3200	611.084	1505.007	1024.821	1536.594	309.450	1490.684	-24.332
3300	612.256	1523.829	1039.659	1597.762	308.726	1527.639	-24.180
3400	613.333	1542.123	1054.170	1659.042	307.806	1564.567	-24.036
3500	614.326	1559.917	1068.367	1720.426	306.692	1601.515	-23.901
3600	615.242	1577.236	1082.262	1781.905	305.398	1638.547	-23.774
3700	616.090	1594.105	1095.869	1843.472	303.906	1675.630	-23.655
3800	616.875	1610.545	1109.198	1905.121	302.197	1712.718	-23.542
3900	617.605	1626.578	1122.259	1966.845	300.299	1749.826	-23.436
4000	618.283	1642.223	1135.063	2028.640	298.199	1787.066	-23.336
4100	618.914	1657.498	1147.620	2090.500	295.879	1824.316	-23.242
4200	619.503	1672.420	1159.938	2152.421	293.353	1861.621	-23.152
4300	620.053	1687.004	1172.027	2214.400	290.613	1898.935	-23.067
4400	620.568	1701.264	1183.894	2276.431	287.665	1936.371	-22.987
4500	621.051	1715.216	1195.546	2338.512	284.518	1973.909	-22.912
4600	621.503	1728.871	1206.992	2400.640	281.139	2011.523	-22.841
4700	621.928	1742.241	1218.239	2462.812	277.539	2049.146	-22.773
4800	622.328	1755.339	1229.293	2525.025	273.745	2086.910	-22.710
4900	622.704	1768.175	1240.160	2587.277	269.713	2124.676	-22.649
5000	623.059	1780.759	1250.846	2649.565	265.498	2162.638	-22.592

3.23. Aceanthrylene



Other names: Cyclopenta[*de*]anthracene

Formula: C₁₆H₁₀

Mass: 202.251 g/mol

CAS Number: 202-03-9

Point Group: C_s

Length: 11.64 Å

Width: 8.578 Å

Breadth: 3.884 Å

L/B Ratio: 1.357

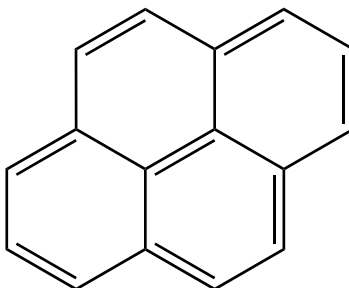
Cartesian coordinates:

C	-2.7714	-1.4524	0.0000	C	-0.3377	-1.7808	0.0000	H	2.1771	-3.0795	0.0000
C	-1.4424	-0.9129	0.0000	C	2.2042	-1.9846	0.0000	H	4.3333	-1.8712	0.0000
C	-1.2954	0.5123	0.0000	C	3.3929	-1.3087	0.0000	H	4.4656	0.6009	0.0000
C	-2.4624	1.3381	0.0000	C	3.4817	0.1222	0.0000	H	-0.4959	-2.8657	0.0000
C	-3.7033	0.7805	0.0000	C	2.3262	0.8406	0.0000	H	-2.3261	2.4257	0.0000
C	-3.8588	-0.6353	0.0000	C	1.9561	2.2655	0.0000	H	-4.6003	1.4083	0.0000
C	-0.0003	1.0303	0.0000	C	0.5968	2.3750	0.0000	H	-4.8714	-1.0517	0.0000
C	1.0775	0.1266	0.0000	H	0.0098	3.2916	0.0000	H	-2.8904	-2.5421	0.0000
C	0.9636	-1.2653	0.0000	H	2.6831	3.0747	0.0000				

Table 3.23: Table of thermodynamic data as a function of temperature for Aceanthrylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-30.549	350.050	350.050	∞
100	66.716	290.507	550.320	-25.981	367.264	390.100	-203.763
200	129.552	354.748	436.524	-16.355	358.204	416.529	-108.784
250	167.230	387.667	423.443	-8.944	353.900	431.609	-90.178
298.15	204.199	420.289	420.289	0.000	350.050	446.934	-78.299
300	205.604	421.556	420.293	0.379	349.908	447.534	-77.921
350	242.537	456.052	422.933	11.592	346.339	464.095	-69.261
400	276.751	490.707	429.239	24.587	343.218	481.130	-62.828
450	307.698	525.123	437.985	39.212	340.490	498.536	-57.867
500	335.327	559.001	448.398	55.301	338.101	516.239	-53.930
600	381.620	624.398	472.330	91.241	334.147	552.257	-48.077
700	418.255	686.083	498.506	131.304	331.152	588.861	-43.940
800	447.703	743.924	525.607	174.653	329.001	625.826	-40.861
900	471.774	798.091	552.907	220.666	327.583	663.013	-38.479
1000	491.723	848.862	579.991	268.871	326.801	700.331	-36.581
1100	508.432	896.535	606.623	318.903	326.533	737.706	-35.030
1200	522.544	941.396	632.670	370.471	326.695	775.076	-33.737
1300	534.544	983.708	658.061	423.341	327.177	812.425	-32.643
1400	544.810	1023.708	682.763	477.322	327.898	849.730	-31.703
1500	553.640	1061.604	706.767	532.255	328.807	886.978	-30.887
1600	561.274	1097.585	730.079	588.010	329.827	924.155	-30.170
1700	567.906	1131.816	752.712	644.477	330.911	961.252	-29.535
1800	573.695	1164.444	774.686	701.563	332.016	998.322	-28.970
1900	578.771	1195.601	796.026	759.192	333.121	1035.300	-28.462
2000	583.240	1225.404	816.755	817.297	334.192	1072.236	-28.003
2100	587.191	1253.958	836.899	875.823	335.183	1109.112	-27.587
2200	590.698	1281.356	856.483	934.721	336.094	1145.944	-27.208
2300	593.823	1307.684	875.532	993.950	336.920	1182.735	-26.860
2400	596.616	1333.017	894.070	1053.474	337.620	1219.466	-26.540
2500	599.123	1357.424	912.119	1113.263	338.199	1256.236	-26.247
2600	601.379	1380.967	929.701	1173.290	338.636	1292.917	-25.974
2700	603.417	1403.702	946.838	1233.532	338.933	1329.626	-25.723
2800	605.262	1425.681	963.549	1293.967	339.076	1366.341	-25.489
2900	606.937	1446.950	979.854	1354.579	339.045	1403.021	-25.271
3000	608.463	1467.552	995.769	1415.350	338.867	1439.720	-25.067
3100	609.856	1487.526	1011.311	1476.267	338.496	1476.384	-24.876
3200	611.131	1506.909	1026.497	1537.317	337.957	1513.105	-24.698
3300	612.300	1525.733	1041.342	1598.490	337.237	1549.869	-24.532
3400	613.376	1544.028	1055.859	1659.774	336.322	1586.608	-24.375
3500	614.366	1561.823	1070.062	1721.162	335.212	1623.364	-24.227
3600	615.280	1579.143	1083.964	1782.645	333.922	1660.206	-24.088
3700	616.126	1596.013	1097.576	1844.216	332.433	1697.099	-23.958
3800	616.910	1612.454	1110.910	1905.868	330.728	1733.996	-23.835
3900	617.637	1628.488	1123.976	1967.596	328.833	1770.912	-23.718
4000	618.314	1644.134	1136.786	2029.394	326.737	1807.961	-23.609
4100	618.944	1659.410	1149.347	2091.257	324.419	1845.021	-23.505
4200	619.531	1674.332	1161.670	2153.181	321.896	1882.135	-23.407
4300	620.080	1688.916	1173.762	2215.162	319.159	1919.258	-23.314
4400	620.594	1703.177	1185.633	2277.196	316.214	1956.502	-23.226
4500	621.075	1717.129	1197.289	2339.280	313.069	1993.849	-23.144
4600	621.527	1730.785	1208.739	2401.410	309.693	2031.271	-23.065
4700	621.951	1744.156	1219.989	2463.584	306.096	2068.703	-22.991
4800	622.350	1757.255	1231.046	2525.799	302.304	2106.275	-22.920
4900	622.725	1770.091	1241.917	2588.053	298.274	2143.849	-22.853
5000	623.079	1782.675	1252.607	2650.343	294.061	2181.620	-22.791

3.24. Pyrene



Other names: Benzo[*def*]phenanthrene

Pyren

Formula: C₁₆H₁₀

Mass: 202.251 g/mol

CAS Number: 129-00-0

Point Group: D_{2h}

Length: 11.60 Å

Width: 9.200 Å

Breadth: 3.884 Å

L/B Ratio: 1.261

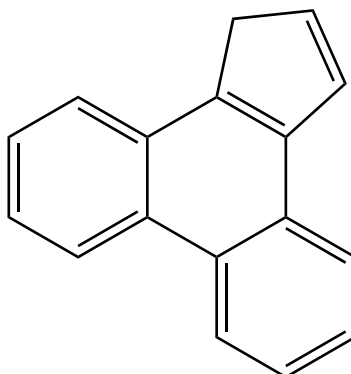
Cartesian coordinates:

C	2.8191	-1.2092	0.0000	C	0.6760	-2.4584	0.0000	H	3.3727	2.1543	0.0000
C	3.5055	-0.0005	0.0000	C	-1.4217	-1.2242	0.0000	H	1.2411	3.3977	0.0000
C	2.8195	1.2084	0.0000	C	-0.7162	0.0001	0.0000	H	-1.2401	3.3980	0.0000
C	1.4217	1.2242	0.0000	C	-1.4214	1.2246	0.0000	H	-1.2412	-3.3977	0.0000
C	0.6766	2.4582	0.0000	C	-2.8192	1.2092	0.0000	H	1.2402	-3.3980	0.0000
C	-0.6759	2.4583	0.0000	C	-3.5055	0.0005	0.0000	H	-3.3722	2.1552	0.0000
C	1.4214	-1.2245	0.0000	C	-2.8195	-1.2084	0.0000	H	-4.6007	0.0006	0.0000
C	0.7162	-0.0001	0.0000	H	3.3722	-2.1552	0.0000	H	-3.3728	-2.1543	0.0000
C	-0.6766	-2.4582	0.0000	H	4.6007	-0.0007	0.0000				

Table 3.24: Table of thermodynamic data as a function of temperature for Pyrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-29.534	231.159	231.159	∞
100	62.084	274.030	526.290	-25.226	243.470	267.954	-139.962
200	125.953	335.323	415.414	-16.018	233.992	296.202	-77.358
250	163.825	367.466	402.589	-8.781	229.513	312.273	-65.244
298.15	200.815	399.491	399.491	0.000	225.500	328.585	-57.566
300	202.220	400.737	399.495	0.373	225.352	329.224	-57.322
350	239.182	434.713	402.093	11.417	221.615	346.839	-51.762
400	273.486	468.925	408.309	24.246	218.327	364.953	-47.657
450	304.585	502.965	416.938	38.712	215.440	383.457	-44.510
500	332.407	536.524	427.224	54.650	212.900	402.277	-42.025
600	379.135	601.427	450.895	90.319	208.676	440.568	-38.354
700	416.194	662.761	476.825	130.155	205.454	479.488	-35.779
800	446.012	720.352	503.705	173.317	203.115	518.799	-33.873
900	470.389	774.338	530.809	219.177	201.545	558.352	-32.405
1000	490.586	824.976	557.720	267.256	200.636	598.052	-31.238
1100	507.493	872.550	584.201	317.184	200.265	637.821	-30.287
1200	521.762	917.337	610.115	368.667	200.342	677.593	-29.494
1300	533.888	959.592	635.388	421.466	200.752	717.351	-28.823
1400	544.255	999.547	659.985	475.386	201.412	757.070	-28.246
1500	553.167	1037.408	683.896	530.268	202.270	796.735	-27.744
1600	560.867	1073.360	707.123	585.979	203.246	836.334	-27.303
1700	567.554	1107.568	729.681	642.408	204.293	875.854	-26.911
1800	573.388	1140.177	751.587	699.461	205.364	915.351	-26.562
1900	578.500	1171.319	772.865	757.061	206.440	954.756	-26.248
2000	583.000	1201.109	793.538	815.141	207.486	994.121	-25.963
2100	586.978	1229.651	813.631	873.644	208.455	1033.426	-25.705
2200	590.507	1257.041	833.167	932.522	209.346	1072.690	-25.468
2300	593.651	1283.361	852.172	991.733	210.154	1111.913	-25.252
2400	596.461	1308.687	870.670	1051.241	210.837	1151.076	-25.052
2500	598.982	1333.087	888.681	1111.015	211.401	1190.280	-24.869
2600	601.251	1356.625	906.229	1171.029	211.825	1229.395	-24.698
2700	603.299	1379.355	923.334	1231.258	212.110	1268.538	-24.541
2800	605.153	1401.330	940.015	1291.682	212.241	1307.688	-24.395
2900	606.838	1422.595	956.291	1352.283	212.200	1346.804	-24.258
3000	608.371	1443.194	972.179	1413.045	212.013	1385.939	-24.131
3100	609.771	1463.166	987.697	1473.953	211.633	1425.038	-24.011
3200	611.051	1482.546	1002.860	1534.995	211.085	1464.196	-23.900
3300	612.226	1501.367	1017.682	1596.159	210.357	1503.396	-23.796
3400	613.306	1519.660	1032.179	1657.437	209.435	1542.571	-23.698
3500	614.301	1537.453	1046.362	1718.818	208.319	1581.765	-23.606
3600	615.219	1554.771	1060.245	1780.294	207.022	1621.044	-23.520
3700	616.068	1571.639	1073.840	1841.859	205.527	1660.373	-23.440
3800	616.855	1588.079	1087.157	1903.506	203.817	1699.708	-23.364
3900	617.586	1604.112	1100.207	1965.229	201.917	1739.062	-23.292
4000	618.265	1619.757	1113.001	2027.022	199.816	1778.549	-23.225
4100	618.898	1635.031	1125.548	2088.880	197.493	1818.046	-23.162
4200	619.488	1649.952	1137.857	2150.800	194.966	1857.597	-23.102
4300	620.039	1664.536	1149.937	2212.776	192.224	1897.159	-23.045
4400	620.555	1678.796	1161.795	2274.806	189.275	1936.841	-22.993
4500	621.038	1692.747	1173.439	2336.886	186.126	1976.626	-22.944
4600	621.491	1706.402	1184.877	2399.013	182.747	2016.487	-22.897
4700	621.917	1719.772	1196.116	2461.183	179.145	2056.356	-22.853
4800	622.317	1732.870	1207.163	2523.395	175.350	2096.367	-22.813
4900	622.694	1745.706	1218.023	2585.646	171.317	2136.380	-22.774
5000	623.049	1758.289	1228.703	2647.933	167.101	2176.589	-22.738

3.25. 1*H*-Cyclopenta[*l*]phenanthrene



Other names: Phenanthrindene
Formula: C₁₇H₁₂
Mass: 216.277 g/mol
CAS Number: 235-92-7
Point Group: C_s

Length: 11.66 Å
Width: 10.29 Å
Breadth: 4.178 Å
L/B Ratio: 1.133

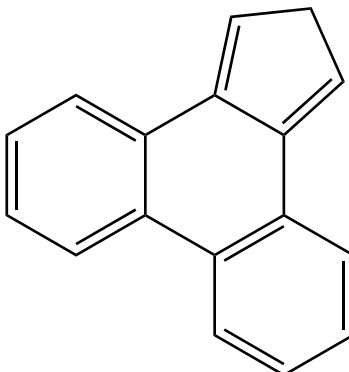
Cartesian coordinates:

C	0.4708	3.0298	0.0011	C	1.9453	-1.8132	-0.0026	H	-1.2231	4.5524	0.0114
C	-1.8021	2.4390	0.0090	C	-1.4477	-0.1565	0.0017	H	3.0073	1.9233	-0.0107
C	-0.9592	3.4970	0.0078	C	-0.4616	-1.1650	-0.0003	H	4.7337	0.1282	-0.0104
C	-1.0140	1.2065	0.0016	C	-0.8755	-2.5147	-0.0005	H	4.0457	-2.2578	-0.0058
C	0.3262	1.5357	-0.0023	C	-2.2120	-2.8432	0.0015	H	1.6329	-2.8688	-0.0017
C	0.9459	-0.8160	-0.0020	C	-3.1882	-1.8340	0.0044	H	-0.1043	-3.3002	-0.0020
C	1.3445	0.5369	-0.0038	C	-2.8128	-0.5097	0.0049	H	-2.5216	-3.8933	0.0012
C	2.7164	0.8666	-0.0079	H	1.0225	3.3890	0.8894	H	-4.2481	-2.1084	0.0062
C	3.6689	-0.1263	-0.0081	H	1.0156	3.3937	-0.8895	H	-3.5695	0.2833	0.0077
C	3.2795	-1.4758	-0.0052	H	-2.8911	2.4592	0.0146				

Table 3.25: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*I*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-34.110	300.372	300.372	∞
100	76.768	301.575	592.104	-29.053	320.975	352.872	-184.317
200	144.943	374.565	465.238	-18.134	310.187	389.047	-101.607
250	185.328	411.199	450.753	-9.888	305.025	409.360	-85.529
298.15	225.398	447.268	447.268	0.000	300.372	429.886	-75.313
300	226.929	448.667	447.272	0.418	300.201	430.690	-74.988
350	267.355	486.711	450.184	12.784	295.866	452.789	-67.574
400	305.053	524.908	457.138	27.108	292.063	475.467	-62.088
450	339.307	562.851	466.780	43.232	288.745	498.595	-57.874
500	369.993	600.219	478.261	60.979	285.854	522.083	-54.540
600	421.619	672.424	504.657	100.660	281.136	569.795	-49.604
700	462.686	740.617	533.544	144.951	277.658	618.200	-46.130
800	495.859	804.642	563.473	192.935	275.266	667.017	-43.551
900	523.094	864.669	593.640	243.926	273.818	716.073	-41.559
1000	545.750	920.990	623.588	297.402	273.179	765.254	-39.972
1100	564.784	973.924	653.055	352.955	273.201	814.471	-38.675
1200	580.900	1023.777	681.892	410.261	273.772	863.650	-37.593
1300	594.631	1070.830	710.018	469.056	274.757	912.771	-36.675
1400	606.396	1115.338	737.394	529.122	276.060	961.807	-35.885
1500	616.529	1157.530	764.009	590.281	277.612	1010.741	-35.196
1600	625.298	1197.606	789.867	652.382	279.323	1059.560	-34.590
1700	632.923	1235.749	814.983	715.302	281.135	1108.252	-34.052
1800	639.582	1272.118	839.377	778.935	282.994	1156.878	-33.571
1900	645.424	1306.858	863.074	843.191	284.876	1205.366	-33.137
2000	650.571	1340.098	886.100	907.997	286.738	1253.772	-32.744
2100	655.123	1371.952	908.482	973.286	288.528	1302.077	-32.387
2200	659.164	1402.523	930.249	1039.004	290.243	1350.302	-32.060
2300	662.766	1431.905	951.425	1105.104	291.876	1398.447	-31.759
2400	665.988	1460.182	972.038	1171.545	293.381	1446.496	-31.482
2500	668.879	1487.428	992.112	1238.291	294.762	1494.556	-31.226
2600	671.482	1513.714	1011.671	1305.311	295.994	1542.490	-30.988
2700	673.832	1539.101	1030.738	1372.578	297.080	1590.422	-30.768
2800	675.961	1563.645	1049.335	1440.070	298.001	1638.335	-30.563
2900	677.895	1587.400	1067.481	1507.764	298.738	1686.182	-30.371
3000	679.656	1610.412	1085.197	1575.643	299.317	1734.022	-30.191
3100	681.264	1632.724	1102.502	1643.690	299.688	1781.800	-30.023
3200	682.736	1654.377	1119.411	1711.892	299.877	1829.614	-29.865
3300	684.086	1675.407	1135.942	1780.234	299.871	1877.449	-29.717
3400	685.328	1695.848	1152.111	1848.705	299.654	1925.236	-29.577
3500	686.471	1715.730	1167.932	1917.296	299.225	1973.019	-29.445
3600	687.527	1735.084	1183.418	1985.996	298.600	2020.869	-29.321
3700	688.504	1753.935	1198.584	2054.799	297.758	2068.756	-29.205
3800	689.409	1772.308	1213.441	2123.695	296.680	2116.625	-29.094
3900	690.249	1790.227	1228.002	2192.678	295.395	2164.497	-28.990
4000	691.030	1807.712	1242.277	2261.743	293.889	2212.491	-28.892
4100	691.758	1824.785	1256.277	2330.882	292.141	2260.478	-28.798
4200	692.437	1841.463	1270.012	2400.093	290.168	2308.504	-28.710
4300	693.071	1857.764	1283.492	2469.368	287.960	2356.523	-28.625
4400	693.665	1873.704	1296.725	2538.705	285.524	2404.657	-28.546
4500	694.221	1889.299	1309.721	2608.100	282.868	2452.885	-28.472
4600	694.742	1904.563	1322.487	2677.548	279.959	2501.176	-28.401
4700	695.232	1919.509	1335.031	2747.047	276.806	2549.461	-28.333
4800	695.693	1934.151	1347.361	2816.594	273.440	2597.882	-28.270
4900	696.127	1948.500	1359.483	2886.185	269.814	2646.292	-28.209
5000	696.536	1962.568	1371.405	2955.818	265.986	2694.899	-28.153

3.26. 2*H*-Cyclopenta[*l*]phenanthrene



Other names: 3,4-(*o,o'*-Biphenylene)cyclopentadiene

Formula: C₁₇H₁₂

Mass: 216.277 g/mol

CAS Number: 235-91-6

Point Group: C_{2v}

Length: 11.67 Å

Width: 9.990 Å

Breadth: 4.178 Å

L/B Ratio: 1.168

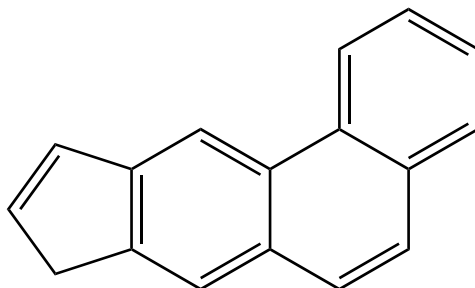
Cartesian coordinates:

C	-2.8292	0.4400	0.0000	C	2.7546	-0.7812	0.0000	H	-0.9230	-4.2218	-0.8893
C	-1.4681	0.1177	0.0000	C	3.6793	0.2526	0.0000	H	3.0970	-1.8225	0.0000
C	-0.5011	1.1426	0.0000	C	3.2415	1.5742	0.0000	H	4.7511	0.0298	0.0000
C	-0.9368	2.4739	0.0000	C	1.8840	1.8569	0.0000	H	3.9695	2.3919	-0.0000
C	-2.2884	2.7837	0.0000	C	-1.7361	-2.4210	0.0000	H	1.5419	2.9031	0.0000
C	-3.2379	1.7654	0.0000	C	-0.7831	-3.5800	-0.0000	H	-0.1892	3.2817	0.0000
C	0.9322	0.8290	0.0000	C	0.5668	-2.9248	0.0000	H	-2.6086	3.8306	0.0000
C	1.3831	-0.5059	0.0000	H	1.4966	-3.4904	0.0000	H	-4.3048	2.0105	0.0000
C	0.4081	-1.5755	0.0000	H	-2.8171	-2.5467	-0.0000	H	-3.5750	-0.3633	0.0000
C	-1.0285	-1.2613	0.0000	H	-0.9230	-4.2218	0.8893				

Table 3.26: Table of thermodynamic data as a function of temperature for 2*H*-Cyclopenta[*I*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-34.414	339.093	339.093	∞
100	77.532	299.415	591.572	-29.216	359.533	391.646	-204.571
200	145.683	372.837	464.012	-18.235	348.807	428.013	-111.783
250	186.366	409.668	449.446	-9.945	343.690	448.407	-93.688
298.15	226.675	445.941	445.941	0.000	339.093	469.003	-82.166
300	228.213	447.348	445.946	0.421	338.924	469.808	-81.799
350	268.785	485.603	448.874	12.855	334.657	491.969	-73.421
400	306.537	523.995	455.866	27.252	330.928	514.697	-67.211
450	340.781	562.113	465.558	43.450	327.684	537.866	-62.433
500	371.414	599.634	477.095	61.270	324.866	561.387	-58.646
600	422.882	672.084	503.609	101.085	320.282	609.145	-53.030
700	463.777	740.460	532.611	145.494	316.921	657.575	-49.068
800	496.794	804.619	562.646	193.579	314.631	706.400	-46.122
900	523.897	864.748	592.908	244.656	313.270	755.453	-43.844
1000	546.442	921.148	622.942	298.207	312.705	804.622	-42.028
1100	565.385	974.144	652.485	353.825	312.791	853.820	-40.544
1200	581.425	1024.045	681.390	411.187	313.419	902.974	-39.305
1300	595.092	1071.138	709.576	470.031	314.453	952.067	-38.254
1400	606.804	1115.679	737.007	530.140	315.799	1001.070	-37.350
1500	616.892	1157.897	763.672	591.338	317.390	1049.968	-36.562
1600	625.623	1197.995	789.574	653.474	319.135	1098.749	-35.870
1700	633.215	1236.156	814.730	716.424	320.978	1147.401	-35.255
1800	639.846	1272.542	839.162	780.085	322.865	1195.986	-34.706
1900	645.664	1307.296	862.893	844.366	324.772	1244.431	-34.211
2000	650.789	1340.547	885.950	909.194	326.657	1292.793	-33.764
2100	655.322	1372.411	908.361	974.505	328.468	1341.052	-33.356
2200	659.348	1402.992	930.154	1040.242	330.202	1389.231	-32.984
2300	662.935	1432.381	951.355	1106.359	331.853	1437.329	-32.642
2400	666.144	1460.665	971.991	1172.816	333.374	1485.329	-32.327
2500	669.023	1487.917	992.086	1239.577	334.770	1533.341	-32.037
2600	671.616	1514.208	1011.665	1306.611	336.016	1581.225	-31.767
2700	673.957	1539.600	1030.751	1373.892	337.115	1629.108	-31.516
2800	676.078	1564.149	1049.365	1441.396	338.048	1676.971	-31.284
2900	678.004	1587.908	1067.528	1509.101	338.796	1724.767	-31.066
3000	679.759	1610.923	1085.260	1576.991	339.385	1772.557	-30.862
3100	681.360	1633.239	1102.578	1645.048	339.766	1820.283	-30.671
3200	682.826	1654.895	1119.501	1713.258	339.965	1868.046	-30.492
3300	684.171	1675.927	1136.046	1781.609	339.968	1915.829	-30.324
3400	685.408	1696.370	1152.227	1850.089	339.758	1963.563	-30.166
3500	686.547	1716.255	1168.059	1918.687	339.338	2011.294	-30.016
3600	687.599	1735.611	1183.557	1987.395	338.720	2059.092	-29.876
3700	688.572	1754.464	1198.733	2056.205	337.885	2106.926	-29.744
3800	689.474	1772.839	1213.600	2125.107	336.814	2154.741	-29.618
3900	690.311	1790.759	1228.170	2194.097	335.535	2202.561	-29.499
4000	691.089	1808.246	1242.455	2263.168	334.035	2250.501	-29.388
4100	691.814	1825.320	1256.463	2332.313	332.293	2298.434	-29.282
4200	692.490	1842.000	1270.207	2401.529	330.325	2346.407	-29.181
4300	693.122	1858.302	1283.695	2470.810	328.122	2394.373	-29.085
4400	693.713	1874.243	1296.936	2540.152	325.691	2442.452	-28.995
4500	694.267	1889.839	1309.939	2609.551	323.040	2490.627	-28.910
4600	694.787	1905.104	1322.712	2679.004	320.136	2538.863	-28.829
4700	695.275	1920.051	1335.263	2748.507	316.987	2587.094	-28.752
4800	695.734	1934.694	1347.599	2818.058	313.626	2635.461	-28.679
4900	696.166	1949.044	1359.727	2887.653	310.003	2683.816	-28.609
5000	696.574	1963.113	1371.655	2957.291	306.179	2732.370	-28.544

3.27. 8*H*-Cyclopenta[*b*]phenanthrene



Formula: C₁₇H₁₂
Mass: 216.277 g/mol
CAS Number: 224-03-3
Point Group: C_s

Length: 13.25 Å
Width: 8.609 Å
Breadth: 4.174 Å
L/B Ratio: 1.539

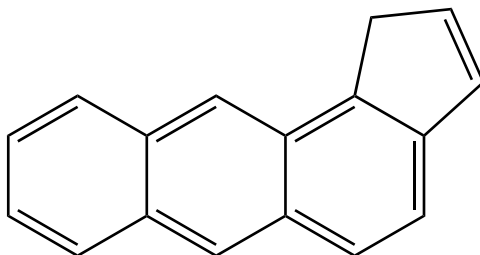
Cartesian coordinates:

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C	4.1204	0.6475	0.0000	C	-1.4982	-0.3886	0.0000	H	2.0049	2.6599	0.0000
C	3.4145	-1.6038	-0.0000	C	-2.4385	0.6567	0.0000	H	0.5523	-2.1594	-0.0000
C	2.2111	-0.7697	-0.0000	C	-3.8181	0.3552	0.0000	H	-0.3212	3.3530	0.0000
C	2.6208	0.5972	0.0000	C	-4.2435	-0.9532	0.0000	H	-2.7430	2.8151	-0.0000
C	1.6986	1.6084	0.0000	C	-3.3063	-2.0003	0.0000	H	-4.5440	1.1763	0.0000
C	0.8829	-1.1103	-0.0000	C	-1.9590	-1.7236	0.0000	H	-5.3129	-1.1875	0.0000
C	-0.0856	-0.0774	-0.0000	H	5.5471	-1.1241	0.0000	H	-3.6570	-3.0374	0.0000
C	0.3218	1.2708	0.0000	H	4.5162	1.1723	0.8887	H	-1.2137	-2.5338	0.0000
C	-0.6664	2.3126	0.0000	H	4.5162	1.1723	-0.8887				

Table 3.27: Table of thermodynamic data as a function of temperature for 8*H*-Cyclopenta[*b*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-34.118	292.892	292.892	∞
100	76.235	303.288	593.532	-29.024	313.523	345.249	-180.336
200	144.757	375.919	466.697	-18.156	302.686	381.275	-99.577
250	185.573	412.558	452.190	-9.908	297.526	401.521	-83.891
298.15	225.936	448.698	448.698	0.000	292.892	421.980	-73.928
300	227.475	450.100	448.702	0.419	292.722	422.781	-73.611
350	268.059	488.242	451.622	12.817	288.419	444.806	-66.382
400	305.815	526.538	458.593	27.178	284.653	467.405	-61.036
450	340.069	564.571	468.260	43.340	281.373	490.449	-56.929
500	370.726	602.018	479.769	61.125	278.520	513.849	-53.680
600	422.272	674.349	506.224	100.875	273.870	561.375	-48.871
700	463.266	742.638	535.170	145.228	270.454	609.583	-45.487
800	496.382	806.735	565.152	193.266	268.118	658.194	-42.975
900	523.573	866.821	595.369	244.307	266.720	707.037	-41.035
1000	546.192	923.191	625.362	297.829	266.127	756.000	-39.489
1100	565.194	976.166	654.870	353.425	266.191	804.995	-38.225
1200	581.281	1026.053	683.744	410.771	266.801	853.948	-37.171
1300	594.985	1073.136	711.903	469.602	267.824	902.840	-36.276
1400	606.724	1117.670	739.311	529.703	269.160	951.644	-35.506
1500	616.834	1159.883	765.954	590.893	270.744	1000.344	-34.834
1600	625.581	1199.978	791.838	653.024	272.484	1048.926	-34.243
1700	633.186	1238.137	816.978	715.971	274.323	1097.380	-33.718
1800	639.827	1274.521	841.394	779.629	276.208	1145.767	-33.249
1900	645.652	1309.274	865.112	843.909	278.114	1194.014	-32.825
2000	650.783	1342.525	888.157	908.736	279.998	1242.178	-32.442
2100	655.320	1374.389	910.557	974.046	281.808	1290.239	-32.092
2200	659.349	1404.969	932.340	1039.783	283.543	1338.220	-31.773
2300	662.939	1434.359	953.533	1105.901	285.194	1386.121	-31.479
2400	666.149	1462.643	974.160	1172.358	286.715	1433.923	-31.208
2500	669.030	1489.896	994.248	1239.120	288.111	1481.737	-30.959
2600	671.624	1516.187	1013.820	1306.155	289.358	1529.424	-30.726
2700	673.966	1541.579	1032.899	1373.436	290.458	1577.108	-30.510
2800	676.087	1566.128	1051.507	1440.941	291.392	1624.774	-30.310
2900	678.014	1589.887	1069.664	1508.647	292.141	1672.372	-30.122
3000	679.769	1612.903	1087.390	1576.538	292.731	1719.963	-29.947
3100	681.370	1635.219	1104.704	1644.596	293.113	1767.492	-29.781
3200	682.836	1656.875	1121.623	1712.807	293.313	1815.056	-29.627
3300	684.181	1677.908	1138.163	1781.159	293.317	1862.642	-29.483
3400	685.418	1698.351	1154.340	1849.640	293.109	1910.177	-29.346
3500	686.557	1718.237	1170.168	1918.240	292.689	1957.710	-29.217
3600	687.609	1737.593	1185.662	1986.949	292.072	2005.310	-29.096
3700	688.581	1756.446	1200.835	2055.759	291.238	2052.946	-28.982
3800	689.483	1774.821	1215.699	2124.662	290.168	2100.563	-28.874
3900	690.320	1792.742	1230.267	2193.653	288.890	2148.184	-28.771
4000	691.098	1810.229	1244.548	2262.724	287.391	2195.927	-28.675
4100	691.822	1827.303	1258.554	2331.871	285.649	2243.661	-28.584
4200	692.499	1843.983	1272.295	2401.087	283.683	2291.436	-28.498
4300	693.130	1860.285	1285.780	2470.369	281.481	2339.203	-28.415
4400	693.721	1876.226	1299.019	2539.712	279.050	2387.084	-28.338
4500	694.275	1891.823	1312.020	2609.112	276.400	2435.060	-28.265
4600	694.794	1907.088	1324.791	2678.566	273.496	2483.098	-28.196
4700	695.282	1922.035	1337.340	2748.070	270.348	2531.131	-28.130
4800	695.741	1936.678	1349.674	2817.621	266.988	2579.300	-28.068
4900	696.173	1951.028	1361.800	2887.217	263.366	2627.456	-28.008
5000	696.580	1965.097	1373.726	2956.855	259.543	2675.812	-27.953

3.28. 1*H*-Cyclopent[*a*]anthracene



Formula: C₁₇H₁₂
Mass: 216.277 g/mol
CAS Number: 227-50-9
Point Group: C_s

Length: 13.11 Å
Width: 8.309 Å
Breadth: 4.177 Å
L/B Ratio: 1.578

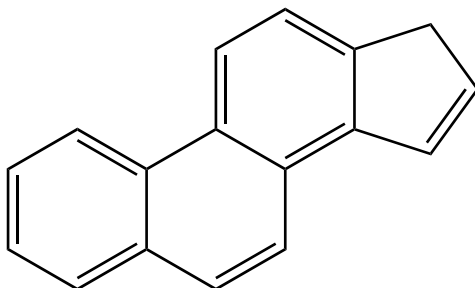
Cartesian coordinates:

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C	-2.1198	-0.6789	0.0000	C	2.9283	-0.4550	0.0000	H	1.0186	-3.2652	0.0000
C	-1.8015	0.7065	0.0000	C	2.6113	-1.8370	0.0000	H	3.4197	-2.5746	0.0000
C	-2.8685	1.6634	0.0000	C	1.2994	-2.2056	0.0000	H	-0.2120	2.1770	0.0000
C	-4.1647	1.2522	0.0000	C	4.2345	0.2014	0.0000	H	-1.3445	-2.6958	0.0000
C	-4.4840	-0.1368	0.0000	C	4.0483	1.5410	0.0000	H	-2.6125	2.7289	0.0000
C	-0.4646	1.1095	0.0000	C	2.5791	1.8709	-0.0000	H	-4.9838	1.9786	0.0000
C	0.5601	0.1609	0.0000	H	2.2932	2.4629	-0.8890	H	-5.5382	-0.4326	0.0000
C	0.2454	-1.2303	0.0000	H	2.2932	2.4629	0.8890	H	-3.7334	-2.1433	0.0000
C	-1.0942	-1.6276	0.0000	H	5.1782	-0.3410	0.0000				

Table 3.28: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopent[*a*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-33.972	315.510	315.510	∞
100	75.583	301.115	590.836	-28.972	336.192	368.136	-192.290
200	144.556	373.444	464.166	-18.144	325.314	404.399	-105.616
250	185.472	410.052	449.666	-9.904	320.147	424.769	-88.749
298.15	225.848	446.176	446.176	0.000	315.510	445.349	-78.022
300	227.387	447.577	446.180	0.419	315.339	446.154	-77.681
350	267.946	485.704	449.098	12.812	311.031	468.307	-69.889
400	305.671	523.983	456.067	27.166	307.259	491.033	-64.121
450	339.905	561.997	465.729	43.321	303.971	514.205	-59.686
500	370.552	599.427	477.234	61.097	301.109	537.734	-56.176
600	422.106	671.726	503.677	100.830	296.443	585.520	-50.973
700	463.125	739.991	532.610	145.167	293.011	633.992	-47.308
800	496.270	804.072	562.581	193.193	290.662	682.868	-44.586
900	523.488	864.147	592.786	244.224	289.254	731.979	-42.482
1000	546.129	920.509	622.770	297.739	288.653	781.210	-40.805
1100	565.149	973.478	652.269	353.330	288.712	830.473	-39.435
1200	581.249	1023.362	681.136	410.672	289.319	879.695	-38.291
1300	594.964	1070.443	709.289	469.500	290.339	928.856	-37.321
1400	606.712	1114.975	736.690	529.599	291.673	977.929	-36.486
1500	616.827	1157.187	763.329	590.788	293.257	1026.899	-35.759
1600	625.578	1197.283	789.208	652.919	294.996	1075.751	-35.119
1700	633.186	1235.442	814.344	715.866	296.835	1124.474	-34.550
1800	639.830	1271.826	838.757	779.524	298.721	1173.130	-34.043
1900	645.656	1306.579	862.472	843.804	300.626	1221.647	-33.585
2000	650.788	1339.830	885.514	908.632	302.511	1270.080	-33.170
2100	655.327	1371.694	907.912	973.942	304.322	1318.411	-32.793
2200	659.356	1402.275	929.693	1039.680	306.057	1366.662	-32.448
2300	662.946	1431.665	950.883	1105.799	307.709	1414.832	-32.131
2400	666.157	1459.949	971.509	1172.257	309.231	1462.903	-31.839
2500	669.038	1487.202	991.595	1239.019	310.628	1510.987	-31.570
2600	671.632	1513.494	1011.165	1306.055	311.876	1558.943	-31.319
2700	673.974	1538.886	1030.243	1373.337	312.976	1606.897	-31.087
2800	676.095	1563.436	1048.849	1440.843	313.911	1654.831	-30.871
2900	678.021	1587.195	1067.006	1508.550	314.660	1702.699	-30.668
3000	679.776	1610.211	1084.731	1576.441	315.252	1750.559	-30.479
3100	681.377	1632.527	1102.044	1644.500	315.635	1798.357	-30.301
3200	682.843	1654.184	1118.961	1712.712	315.835	1846.191	-30.135
3300	684.188	1675.217	1135.500	1781.065	315.839	1894.045	-29.980
3400	685.424	1695.660	1151.676	1849.546	315.632	1941.850	-29.832
3500	686.563	1715.546	1167.504	1918.146	315.213	1989.652	-29.693
3600	687.615	1734.902	1182.998	1986.856	314.596	2037.521	-29.563
3700	688.587	1753.755	1198.170	2055.666	313.763	2085.426	-29.440
3800	689.488	1772.131	1213.033	2124.571	312.693	2133.312	-29.324
3900	690.325	1790.052	1227.600	2193.562	311.416	2181.202	-29.213
4000	691.103	1807.539	1241.881	2262.634	309.917	2229.213	-29.110
4100	691.827	1824.613	1255.886	2331.781	308.176	2277.217	-29.012
4200	692.503	1841.293	1269.627	2400.998	306.210	2325.261	-28.918
4300	693.135	1857.595	1283.111	2470.280	304.009	2373.297	-28.829
4400	693.726	1873.537	1296.350	2539.623	301.579	2421.447	-28.746
4500	694.279	1889.133	1309.350	2609.024	298.928	2469.692	-28.667
4600	694.798	1904.398	1322.120	2678.478	296.026	2517.999	-28.592
4700	695.286	1919.346	1334.669	2747.982	292.878	2566.301	-28.521
4800	695.745	1933.989	1347.003	2817.534	289.518	2614.738	-28.454
4900	696.177	1948.339	1359.129	2887.131	285.896	2663.164	-28.389
5000	696.584	1962.408	1371.054	2956.769	282.073	2711.788	-28.329

3.29. 1*H*-Cyclopenta[*a*]phenanthrene



Other names: 1,2-Cyclo- δ 1',4'-pentadienophenanthrene

Formula: C₁₇H₁₂

Mass: 216.277 g/mol

CAS Number: 219-08-9

Point Group: C_s

Length: 12.99 Å

Width: 7.960 Å

Breadth: 4.175 Å

L/B Ratio: 1.632

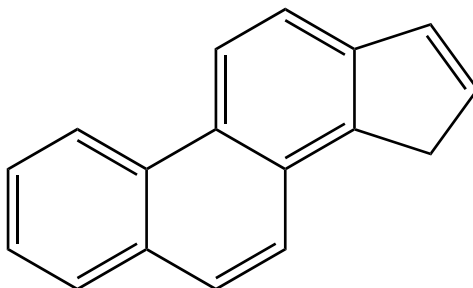
Cartesian coordinates:

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C	-4.3455	0.6253	0.0000	C	2.1213	0.9817	0.0000	H	-2.1619	-3.0486	0.0000
C	-4.0824	-0.8569	0.0000	C	1.6051	-0.3263	-0.0000	H	0.3134	-2.6846	-0.0000
C	-2.0651	0.3776	-0.0000	C	2.5035	-1.4151	0.0000	H	1.6571	3.1121	0.0000
C	-2.5842	-0.9244	0.0000	C	3.8631	-1.2037	0.0000	H	-0.8036	2.7748	-0.0000
C	-1.7439	-2.0374	0.0000	C	4.3751	0.1042	0.0000	H	2.0903	-2.4353	-0.0000
C	-0.3790	-1.8286	-0.0000	C	3.5186	1.1815	0.0000	H	4.5537	-2.0532	0.0000
C	-0.6768	0.6002	-0.0000	H	-3.0632	2.4017	-0.0000	H	5.4590	0.2588	0.0000
C	0.1713	-0.5278	-0.0000	H	-5.3556	1.0301	0.0000	H	3.9120	2.2044	0.0000
C	1.2254	2.1047	0.0000	H	-4.5184	-1.3480	0.8892				

Table 3.29: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-34.211	297.811	297.811	∞
100	76.769	303.637	594.458	-29.082	318.384	350.075	-182.857
200	145.058	376.564	467.424	-18.172	307.588	386.048	-100.823
250	185.736	413.256	452.906	-9.913	302.439	406.260	-84.882
298.15	225.971	449.413	449.413	0.000	297.811	426.685	-74.752
300	227.506	450.815	449.417	0.419	297.640	427.485	-74.430
350	267.995	488.954	452.337	12.816	293.336	449.475	-67.079
400	305.694	527.237	459.307	27.172	289.566	472.038	-61.641
450	339.919	565.254	468.971	43.327	286.279	495.047	-57.462
500	370.564	602.685	480.477	61.104	283.418	518.413	-54.157
600	422.108	674.986	506.923	100.838	278.752	565.874	-49.263
700	463.107	743.250	535.858	145.175	275.320	614.019	-45.818
800	496.227	807.327	565.830	193.198	272.968	662.570	-43.261
900	523.421	867.395	596.036	244.223	271.554	711.356	-41.285
1000	546.043	923.749	626.019	297.730	270.946	760.262	-39.711
1100	565.050	976.709	655.517	353.312	270.996	809.202	-38.425
1200	581.141	1026.584	684.382	410.643	271.592	858.101	-37.351
1300	594.851	1073.656	712.532	469.461	272.601	906.941	-36.441
1400	606.597	1118.180	739.932	529.548	273.924	955.693	-35.657
1500	616.713	1160.384	766.567	590.726	275.496	1004.342	-34.974
1600	625.467	1200.472	792.444	652.845	277.224	1052.875	-34.372
1700	633.078	1238.625	817.577	715.781	279.052	1101.280	-33.838
1800	639.726	1275.003	841.987	779.429	280.927	1149.618	-33.360
1900	645.557	1309.751	865.698	843.699	282.822	1197.817	-32.930
2000	650.693	1342.997	888.738	908.517	284.697	1245.934	-32.540
2100	655.237	1374.856	911.133	973.818	286.499	1293.948	-32.185
2200	659.270	1405.433	932.911	1039.547	288.225	1341.883	-31.860
2300	662.865	1434.819	954.099	1105.657	289.868	1389.737	-31.561
2400	666.080	1463.100	974.722	1172.108	291.383	1437.493	-31.286
2500	668.965	1490.350	994.805	1238.862	292.772	1485.262	-31.032
2600	671.562	1516.639	1014.373	1305.891	294.013	1532.903	-30.796
2700	673.908	1542.029	1033.448	1373.166	295.106	1580.543	-30.577
2800	676.032	1566.576	1052.053	1440.665	296.035	1628.163	-30.373
2900	677.962	1590.333	1070.207	1508.366	296.778	1675.717	-30.182
3000	679.719	1613.347	1087.930	1576.252	297.364	1723.264	-30.004
3100	681.324	1635.662	1105.240	1644.305	297.741	1770.748	-29.836
3200	682.792	1657.316	1122.156	1712.512	297.936	1818.268	-29.680
3300	684.139	1678.348	1138.693	1780.860	297.936	1865.809	-29.533
3400	685.378	1698.790	1154.868	1849.336	297.723	1913.301	-29.394
3500	686.519	1718.674	1170.694	1917.932	297.300	1960.790	-29.263
3600	687.573	1738.029	1186.185	1986.637	296.679	2008.346	-29.140
3700	688.547	1756.881	1201.356	2055.444	295.842	2055.939	-29.024
3800	689.450	1775.256	1216.218	2124.344	294.768	2103.513	-28.914
3900	690.288	1793.175	1230.783	2193.332	293.487	2151.090	-28.810
4000	691.068	1810.662	1245.062	2262.400	291.985	2198.789	-28.713
4100	691.794	1827.735	1259.066	2331.544	290.240	2246.481	-28.620
4200	692.471	1844.414	1272.805	2400.757	288.271	2294.212	-28.532
4300	693.104	1860.716	1286.289	2470.036	286.066	2341.936	-28.448
4400	693.696	1876.657	1299.526	2539.377	283.634	2389.774	-28.370
4500	694.251	1892.252	1312.525	2608.774	280.980	2437.707	-28.296
4600	694.771	1907.517	1325.294	2678.226	278.075	2485.702	-28.225
4700	695.260	1922.464	1337.841	2747.727	274.924	2533.692	-28.158
4800	695.719	1937.107	1350.174	2817.277	271.562	2581.818	-28.095
4900	696.152	1951.456	1362.299	2886.870	267.937	2629.932	-28.035
5000	696.560	1965.525	1374.223	2956.506	264.112	2678.244	-27.979

3.30. 1*H*-Cyclopenta[*a*]phenanthrene



Other names: 1,2-Cyclo- δ 1',3'-pentadienophenanthrene

Formula: C₁₇H₁₂

Mass: 216.277 g/mol

CAS Number: 219-07-8

Point Group: C_s

Length: 13.08 Å

Width: 7.962 Å

Breadth: 4.176 Å

L/B Ratio: 1.643

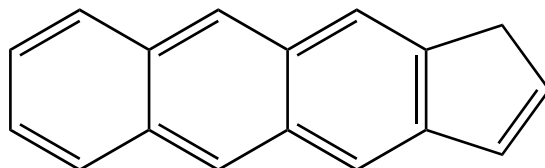
Cartesian coordinates:

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C	-4.4144	0.4272	-0.0000	C	2.1109	0.9910	0.0000	H	-2.1468	-3.0687	0.0000
C	-4.0416	-0.8714	0.0000	C	1.6050	-0.3212	0.0000	H	0.3295	-2.6898	0.0000
C	-2.0665	0.3579	-0.0000	C	2.5116	-1.4032	-0.0000	H	1.6312	3.1184	0.0000
C	-2.5804	-0.9452	0.0000	C	3.8696	-1.1813	-0.0000	H	-0.8310	2.7589	0.0000
C	-1.7317	-2.0562	0.0000	C	4.3714	0.1305	-0.0000	H	2.1055	-2.4263	-0.0000
C	-0.3694	-1.8391	0.0000	C	3.5066	1.2013	0.0000	H	4.5668	-2.0254	-0.0000
C	-0.6829	0.5878	0.0000	H	-3.1928	1.9879	-0.8889	H	5.4540	0.2936	-0.0000
C	0.1731	-0.5344	0.0000	H	-3.1928	1.9879	0.8889	H	3.8923	2.2272	0.0000
C	1.2067	2.1078	0.0000	H	-5.4287	0.8214	-0.0000				

Table 3.30: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-34.245	297.183	297.183	∞
100	76.869	303.747	594.856	-29.111	317.727	349.407	-182.508
200	145.191	376.744	467.697	-18.191	306.941	385.365	-100.645
250	185.927	413.473	453.164	-9.923	301.801	405.567	-84.737
298.15	226.208	449.667	449.667	0.000	297.183	425.981	-74.629
300	227.744	451.071	449.671	0.420	297.013	426.780	-74.307
350	268.260	489.249	452.594	12.829	292.721	448.756	-66.972
400	305.969	527.568	459.572	27.199	288.964	471.304	-61.545
450	340.192	565.618	469.245	43.368	285.691	494.296	-57.375
500	370.828	603.077	480.761	61.158	282.844	517.643	-54.077
600	422.344	675.424	507.229	100.917	278.203	565.062	-49.192
700	463.315	743.722	536.185	145.276	274.792	613.162	-45.754
800	496.409	807.825	566.177	193.318	272.460	661.664	-43.201
900	523.582	867.913	596.401	244.361	271.063	710.399	-41.230
1000	546.187	924.283	626.400	297.883	270.471	759.253	-39.658
1100	565.178	977.256	655.913	353.478	270.534	808.139	-38.375
1200	581.256	1027.142	684.790	410.822	271.142	856.983	-37.303
1300	594.955	1074.222	712.953	469.650	272.162	905.766	-36.393
1400	606.691	1118.754	740.363	529.747	273.495	954.461	-35.611
1500	616.799	1160.964	767.008	590.934	275.076	1003.052	-34.929
1600	625.545	1201.057	792.894	653.062	276.812	1051.527	-34.328
1700	633.150	1239.214	818.035	716.005	278.648	1099.873	-33.794
1800	639.791	1275.596	842.452	779.659	280.529	1148.152	-33.318
1900	645.617	1310.347	866.171	843.936	282.431	1196.292	-32.888
2000	650.749	1343.596	889.217	908.760	284.311	1244.348	-32.498
2100	655.288	1375.459	911.618	974.066	286.119	1292.303	-32.144
2200	659.318	1406.038	933.401	1039.800	287.850	1340.177	-31.819
2300	662.909	1435.426	954.593	1105.915	289.498	1387.971	-31.521
2400	666.121	1463.708	975.221	1172.370	291.016	1435.667	-31.246
2500	669.003	1490.960	995.309	1239.128	292.410	1483.374	-30.993
2600	671.598	1517.250	1014.881	1306.161	293.654	1530.954	-30.757
2700	673.942	1542.642	1033.960	1373.440	294.751	1578.532	-30.538
2800	676.064	1567.190	1052.568	1440.942	295.683	1626.092	-30.334
2900	677.992	1590.948	1070.726	1508.646	296.430	1673.584	-30.144
3000	679.747	1613.963	1088.452	1576.534	297.018	1721.069	-29.966
3100	681.350	1636.279	1105.766	1644.590	297.398	1768.492	-29.798
3200	682.817	1657.934	1122.684	1712.800	297.595	1815.950	-29.642
3300	684.163	1678.966	1139.224	1781.150	297.597	1863.429	-29.495
3400	685.400	1699.409	1155.401	1849.629	297.387	1910.860	-29.356
3500	686.540	1719.294	1171.229	1918.227	296.966	1958.286	-29.225
3600	687.592	1738.649	1186.723	1986.934	296.347	2005.781	-29.103
3700	688.566	1757.502	1201.896	2055.742	295.512	2053.311	-28.987
3800	689.468	1775.877	1216.760	2124.645	294.440	2100.823	-28.877
3900	690.305	1793.797	1231.327	2193.634	293.160	2148.338	-28.773
4000	691.084	1811.284	1245.608	2262.704	291.660	2195.975	-28.676
4100	691.809	1828.358	1259.614	2331.849	289.918	2243.604	-28.583
4200	692.486	1845.037	1273.355	2401.064	287.950	2291.273	-28.496
4300	693.118	1861.339	1286.840	2470.345	285.746	2338.935	-28.412
4400	693.710	1877.281	1300.079	2539.686	283.315	2386.711	-28.333
4500	694.264	1892.876	1313.080	2609.085	280.663	2434.581	-28.259
4600	694.784	1908.141	1325.851	2678.538	277.759	2482.514	-28.189
4700	695.272	1923.089	1338.399	2748.041	274.610	2530.441	-28.122
4800	695.731	1937.732	1350.733	2817.591	271.248	2578.505	-28.059
4900	696.164	1952.081	1362.860	2887.186	267.625	2626.556	-27.999
5000	696.571	1966.150	1374.785	2956.823	263.801	2674.806	-27.943

3.31. 1*H*-Cyclopent[*b*]anthracene



Formula: C₁₇H₁₂
Mass: 216.277 g/mol
CAS Number: 259-06-3
Point Group: C_s

Length: 13.92 Å
Width: 7.442 Å
Breadth: 4.174 Å
L/B Ratio: 1.870

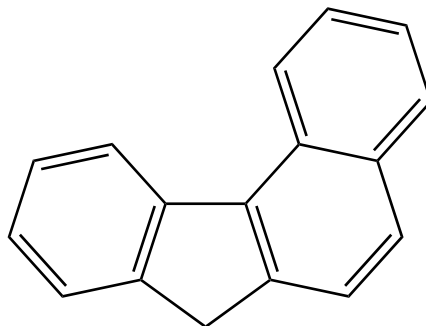
Cartesian coordinates:

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C	-4.8852	0.0537	0.0000	C	2.1507	0.7306	0.0000	H	-1.4871	-2.5329	0.0000
C	-4.0909	-1.2262	0.0000	C	2.1618	-0.6894	0.0000	H	-1.5312	2.5146	0.0000
C	-2.6813	0.7024	0.0000	C	3.4203	-1.3732	0.0000	H	0.9635	-2.4886	0.0000
C	-2.6700	-0.7437	0.0000	C	4.5866	-0.6726	0.0000	H	0.9239	2.5106	0.0000
C	-1.5077	-1.4380	0.0000	C	4.5754	0.7518	0.0000	H	3.4190	-2.4690	0.0000
C	-1.5295	1.4195	0.0000	C	3.3983	1.4341	0.0000	H	5.5513	-1.1902	0.0000
C	-0.2773	0.7141	0.0000	H	-4.3773	2.1832	0.0000	H	5.5319	1.2846	0.0000
C	-0.2659	-0.7116	0.0000	H	-5.9739	0.0470	0.0000	H	3.3797	2.5298	0.0000
C	0.9524	-1.3916	0.0000	H	-4.3178	-1.8439	0.8883				

Table 3.31: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopent[*b*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-34.056	310.757	310.757	∞
100	75.767	302.337	592.433	-29.010	331.403	363.224	-189.725
200	144.728	374.810	465.616	-18.161	320.545	399.356	-104.299
250	185.643	411.455	451.103	-9.912	315.386	419.657	-87.681
298.15	226.030	447.610	447.610	0.000	310.757	440.169	-77.114
300	227.569	449.012	447.614	0.420	310.587	440.972	-76.778
350	268.121	487.167	450.535	12.821	306.288	463.052	-69.105
400	305.824	525.468	457.508	27.184	302.524	485.704	-63.425
450	340.026	563.499	467.176	43.345	299.243	508.801	-59.059
500	370.643	600.939	478.686	61.126	296.387	532.255	-55.603
600	422.152	673.251	505.140	100.866	291.727	579.890	-50.483
700	463.151	741.521	534.083	145.207	288.298	628.208	-46.877
800	496.292	805.605	564.061	193.235	285.952	676.932	-44.198
900	523.514	865.682	594.272	244.269	284.546	725.889	-42.129
1000	546.162	922.047	624.261	297.786	283.948	774.966	-40.479
1100	565.188	975.020	653.765	353.381	284.011	824.075	-39.131
1200	581.292	1024.907	682.635	410.726	284.622	873.143	-38.006
1300	595.010	1071.992	710.792	469.560	285.646	922.150	-37.052
1400	606.759	1116.528	738.197	529.663	286.985	971.068	-36.230
1500	616.875	1158.743	764.839	590.857	288.573	1019.881	-35.515
1600	625.626	1198.842	790.721	652.992	290.318	1068.578	-34.885
1700	633.233	1237.004	815.860	715.944	292.161	1117.145	-34.325
1800	639.876	1273.390	840.275	779.607	294.051	1165.645	-33.825
1900	645.701	1308.146	863.992	843.892	295.961	1214.005	-33.375
2000	650.831	1341.399	887.037	908.724	297.850	1262.282	-32.967
2100	655.368	1373.266	909.438	974.039	299.666	1310.456	-32.595
2200	659.395	1403.848	931.220	1039.781	301.405	1358.549	-32.255
2300	662.984	1433.240	952.413	1105.903	303.060	1406.561	-31.943
2400	666.193	1461.525	973.040	1172.365	304.586	1454.475	-31.655
2500	669.072	1488.780	993.128	1239.130	305.987	1502.401	-31.390
2600	671.664	1515.073	1012.700	1306.169	307.238	1550.199	-31.143
2700	674.004	1540.466	1031.779	1373.455	308.341	1597.995	-30.914
2800	676.124	1565.017	1050.388	1440.963	309.279	1645.772	-30.702
2900	678.049	1588.777	1068.545	1508.673	310.031	1693.481	-30.502
3000	679.802	1611.794	1086.272	1576.567	310.625	1741.183	-30.316
3100	681.402	1634.111	1103.586	1644.629	311.011	1788.823	-30.141
3200	682.867	1655.769	1120.505	1712.843	311.213	1836.498	-29.977
3300	684.211	1676.802	1137.045	1781.198	311.220	1884.194	-29.824
3400	685.446	1697.247	1153.223	1849.682	311.015	1931.840	-29.678
3500	686.584	1717.133	1169.052	1918.284	310.598	1979.483	-29.542
3600	687.634	1736.489	1184.546	1986.995	309.984	2027.193	-29.413
3700	688.606	1755.343	1199.719	2055.808	309.152	2074.940	-29.292
3800	689.506	1773.719	1214.584	2124.714	308.085	2122.667	-29.177
3900	690.342	1791.640	1229.151	2193.707	306.809	2170.398	-29.069
4000	691.120	1809.128	1243.433	2262.781	305.312	2218.251	-28.967
4100	691.843	1826.203	1257.440	2331.929	303.573	2266.096	-28.870
4200	692.519	1842.883	1271.181	2401.148	301.608	2313.980	-28.778
4300	693.150	1859.186	1284.667	2470.432	299.408	2361.857	-28.690
4400	693.740	1875.128	1297.906	2539.776	296.980	2409.848	-28.608
4500	694.293	1890.724	1310.907	2609.178	294.331	2457.934	-28.530
4600	694.812	1905.990	1323.678	2678.634	291.429	2506.082	-28.457
4700	695.299	1920.938	1336.227	2748.140	288.283	2554.225	-28.386
4800	695.757	1935.581	1348.562	2817.693	284.924	2602.503	-28.320
4900	696.188	1949.931	1360.689	2887.290	281.303	2650.769	-28.257
5000	696.595	1964.001	1372.615	2956.929	277.482	2699.234	-28.198

3.32. 7H-Benzo[*c*]fluorene



Other names: Benzo[*c*]fluorene
3,4-Benzofluorene
Isochrysofluorene

Formula: C₁₇H₁₂
Mass: 216.277 g/mol
CAS Number: 205-12-9
Point Group: C_s

Length: 12.47 Å
Width: 9.171 Å
Breadth: 4.177 Å
L/B Ratio: 1.360

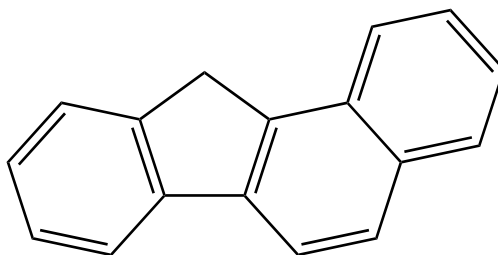
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C	2.3152	0.7912	0.0000	C	-1.2403	-0.3362	0.0000	H	5.2063	-0.9608	-0.0000
C	1.3913	-0.2836	0.0000	C	-2.3768	0.5092	0.0000	H	4.3865	1.3963	-0.0000
C	1.8525	-1.5912	0.0000	C	-3.6758	-0.0716	0.0000	H	-0.8619	3.5895	0.0000
C	3.2293	-1.8178	0.0000	C	-3.8301	-1.4300	-0.0000	H	-3.1300	2.5458	0.0000
C	4.1301	-0.7590	0.0000	C	-2.6959	-2.2750	-0.0000	H	-4.5493	0.5906	0.0000
C	3.6783	0.5621	-0.0000	C	-1.4356	-1.7442	0.0000	H	-4.8288	-1.8786	-0.0000
C	0.0370	0.2791	0.0000	H	1.8301	2.7110	0.8889	H	-2.8417	-3.3602	-0.0000
C	0.1457	1.6705	0.0000	H	1.8301	2.7110	-0.8889	H	-0.5556	-2.4024	0.0000
C	-0.9849	2.5019	0.0000	H	1.1503	-2.4354	0.0000				

Table 3.32: Table of thermodynamic data as a function of temperature for 7*H*-Benzo[*c*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-34.210	266.341	266.341	∞
100	77.135	307.574	597.137	-28.956	287.040	318.337	-166.279
200	144.332	380.339	470.718	-18.076	276.214	353.920	-92.432
250	184.734	416.838	456.277	-9.860	271.022	373.947	-78.130
298.15	224.802	452.802	452.802	0.000	266.341	394.205	-69.062
300	226.332	454.197	452.806	0.417	266.168	394.998	-68.774
350	266.752	492.149	455.711	12.753	261.803	416.824	-62.206
400	304.458	530.266	462.649	27.047	257.971	439.231	-57.357
450	338.738	568.140	472.270	43.142	254.624	462.093	-53.637
500	369.462	605.451	483.728	60.861	251.705	485.318	-50.700
600	421.181	677.566	510.076	100.494	246.938	532.512	-46.358
700	462.342	745.699	538.920	144.746	243.421	580.406	-43.310
800	495.597	809.683	568.809	192.700	241.000	628.717	-41.050
900	522.898	869.683	598.942	243.667	239.529	677.270	-39.307
1000	545.606	925.987	628.860	297.127	238.873	725.951	-37.919
1100	564.681	978.909	658.302	352.668	238.882	774.669	-36.785
1200	580.826	1028.754	687.116	409.965	239.444	823.350	-35.839
1300	594.580	1075.803	715.223	468.754	240.424	871.973	-35.036
1400	606.362	1120.308	742.583	528.816	241.722	920.512	-34.344
1500	616.507	1162.497	769.183	589.971	243.272	968.949	-33.741
1600	625.286	1202.573	795.028	652.071	244.981	1017.271	-33.210
1700	632.917	1240.715	820.132	714.990	246.791	1065.466	-32.737
1800	639.582	1277.084	844.516	778.623	248.651	1113.596	-32.315
1900	645.428	1311.824	868.204	842.879	250.533	1161.588	-31.934
2000	650.577	1345.064	891.222	907.685	252.395	1209.497	-31.588
2100	655.131	1376.918	913.597	972.975	254.186	1257.305	-31.273
2200	659.174	1407.490	935.356	1038.694	255.902	1305.034	-30.985
2300	662.777	1436.873	956.527	1104.795	257.536	1352.682	-30.720
2400	665.999	1465.149	977.134	1171.237	259.042	1400.234	-30.475
2500	668.890	1492.397	997.203	1237.984	260.424	1447.798	-30.249
2600	671.493	1518.682	1016.757	1305.005	261.657	1495.234	-30.039
2700	673.844	1544.070	1035.820	1372.274	262.744	1542.669	-29.844
2800	675.973	1568.615	1054.412	1439.767	263.667	1590.086	-29.663
2900	677.907	1592.370	1072.555	1507.462	264.404	1637.436	-29.493
3000	679.668	1615.382	1090.268	1575.342	264.984	1684.779	-29.334
3100	681.275	1637.695	1107.569	1643.391	265.357	1732.060	-29.184
3200	682.747	1659.348	1124.475	1711.593	265.547	1779.377	-29.045
3300	684.097	1680.378	1141.004	1779.936	265.542	1826.715	-28.914
3400	685.338	1700.819	1157.170	1848.408	265.326	1874.004	-28.790
3500	686.481	1720.702	1172.988	1917.000	264.898	1921.290	-28.673
3600	687.537	1740.056	1188.472	1985.702	264.274	1968.643	-28.564
3700	688.513	1758.907	1203.636	2054.505	263.433	2016.033	-28.461
3800	689.418	1777.281	1218.491	2123.402	262.356	2063.404	-28.363
3900	690.258	1795.200	1233.050	2192.386	261.071	2110.779	-28.270
4000	691.039	1812.686	1247.323	2261.452	259.567	2158.276	-28.184
4100	691.766	1829.758	1261.321	2330.592	257.819	2205.765	-28.101
4200	692.445	1846.436	1275.055	2399.803	255.847	2253.294	-28.023
4300	693.079	1862.737	1288.533	2469.080	253.640	2300.816	-27.949
4400	693.672	1878.678	1301.765	2538.418	251.205	2348.452	-27.879
4500	694.228	1894.273	1314.759	2607.813	248.549	2396.183	-27.814
4600	694.749	1909.537	1327.524	2677.262	245.641	2443.976	-27.752
4700	695.239	1924.484	1340.066	2746.762	242.489	2491.764	-27.692
4800	695.699	1939.126	1352.395	2816.309	239.124	2539.688	-27.637
4900	696.133	1953.475	1364.516	2885.901	235.498	2587.600	-27.584
5000	696.542	1967.543	1376.436	2955.534	231.671	2635.710	-27.535

3.33. 1*H*-Benzo[*a*]fluorene



Other names: Benzo[*a*]fluorene
1,2-Benzofluorene
Chrysofluorene

Formula: C₁₇H₁₂

Mass: 216.277 g/mol

CAS Number: 238-84-6

Point Group: C_s

Length: 13.38 Å

Width: 7.963 Å

Breadth: 4.176 Å

L/B Ratio: 1.681

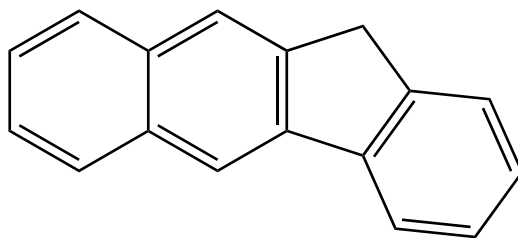
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C	1.8902	0.5585	0.0000	C	-1.6243	-0.4775	0.0000	H	5.1141	1.5729	0.0000
C	2.0964	-0.8420	0.0000	C	-2.3319	0.7480	0.0000	H	2.8005	2.5172	0.0000
C	3.3759	-1.3651	0.0000	C	-3.7542	0.7195	0.0000	H	0.2920	2.9679	0.0000
C	4.4547	-0.4775	0.0000	C	-4.4242	-0.4729	0.0000	H	-2.2068	2.9153	0.0000
C	4.2514	0.8985	0.0000	C	-3.7129	-1.6967	0.0000	H	-4.3012	1.6692	0.0000
C	2.9626	1.4346	0.0000	C	-2.3456	-1.7023	0.0000	H	-5.5189	-0.4955	0.0000
C	-0.2134	-0.4213	0.0000	H	0.6552	-2.2034	0.8888	H	-4.2735	-2.6372	0.0000
C	0.4496	0.8044	0.0000	H	0.6552	-2.2034	-0.8888	H	-1.7826	-2.6426	0.0000
C	-0.2571	2.0206	0.0000	H	3.5407	-2.4468	0.0000				

Table 3.33: Table of thermodynamic data as a function of temperature for 1*H*-Benzo[*a*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-33.773	256.751	256.751	∞
100	75.872	302.100	589.253	-28.715	277.690	309.535	-161.681
200	143.095	374.029	463.806	-17.955	266.744	345.712	-90.289
250	183.502	410.251	449.457	-9.801	261.490	366.062	-76.483
298.15	223.612	446.002	446.002	0.000	256.751	386.642	-67.737
300	225.144	447.390	446.006	0.415	256.576	387.447	-67.459
350	265.628	485.163	448.897	12.693	252.153	409.618	-61.131
400	303.410	523.135	455.804	26.932	248.266	432.379	-56.462
450	337.771	560.890	465.386	42.977	244.868	455.600	-52.884
500	368.579	598.103	476.803	60.650	241.904	479.190	-50.060
600	420.467	670.073	503.068	100.203	237.057	527.127	-45.890
700	461.783	738.108	531.834	144.392	233.476	575.775	-42.964
800	495.171	802.026	561.656	192.296	231.006	624.849	-40.798
900	522.582	861.983	591.730	243.227	229.498	674.170	-39.127
1000	545.376	918.258	621.599	296.659	228.815	723.622	-37.797
1100	564.517	971.161	650.997	352.181	228.804	773.114	-36.711
1200	580.713	1020.994	679.774	409.464	229.353	822.570	-35.805
1300	594.505	1068.035	707.848	468.243	230.323	871.970	-35.035
1400	606.315	1112.536	735.179	528.299	231.615	921.286	-34.373
1500	616.481	1154.723	761.755	589.452	233.161	970.500	-33.795
1600	625.275	1194.797	787.578	651.550	234.869	1019.600	-33.286
1700	632.918	1232.939	812.663	714.469	236.679	1068.573	-32.833
1800	639.591	1269.308	837.030	778.101	238.539	1117.480	-32.428
1900	645.443	1304.050	860.702	842.360	240.422	1166.249	-32.062
2000	650.597	1337.290	883.707	907.167	242.286	1214.936	-31.730
2100	655.153	1369.145	906.070	972.459	244.080	1263.522	-31.428
2200	659.199	1399.718	927.818	1038.181	245.798	1312.027	-31.151
2300	662.803	1429.102	948.978	1104.284	247.435	1360.453	-30.896
2400	666.026	1457.380	969.576	1170.728	248.943	1408.781	-30.661
2500	668.917	1484.628	989.637	1237.478	250.328	1457.122	-30.444
2600	671.520	1510.915	1009.183	1304.502	251.564	1505.336	-30.242
2700	673.871	1536.303	1028.239	1371.774	252.653	1553.548	-30.055
2800	675.999	1560.849	1046.825	1439.269	253.578	1601.741	-29.880
2900	677.932	1584.605	1064.962	1506.967	254.319	1649.867	-29.717
3000	679.693	1607.619	1082.669	1574.850	254.901	1697.987	-29.564
3100	681.300	1629.932	1099.964	1642.900	255.276	1746.044	-29.420
3200	682.770	1651.586	1116.866	1711.105	255.469	1794.137	-29.286
3300	684.120	1672.617	1133.390	1779.450	255.466	1842.251	-29.160
3400	685.360	1693.059	1149.551	1847.925	255.252	1890.316	-29.041
3500	686.503	1712.942	1165.365	1916.519	254.827	1938.378	-28.928
3600	687.557	1732.297	1180.846	1985.223	254.204	1986.508	-28.823
3700	688.533	1751.148	1196.006	2054.028	253.366	2034.673	-28.724
3800	689.437	1769.523	1210.858	2122.927	252.291	2082.821	-28.630
3900	690.276	1787.442	1225.413	2191.913	251.008	2130.971	-28.541
4000	691.057	1804.928	1239.683	2260.980	249.505	2179.244	-28.457
4100	691.784	1822.001	1253.679	2330.123	247.759	2227.509	-28.378
4200	692.462	1838.680	1267.409	2399.336	245.789	2275.814	-28.303
4300	693.095	1854.981	1280.885	2468.614	243.583	2324.111	-28.232
4400	693.688	1870.922	1294.115	2537.953	241.150	2372.522	-28.165
4500	694.243	1886.518	1307.106	2607.350	238.496	2421.029	-28.102
4600	694.764	1901.782	1319.869	2676.801	235.589	2469.598	-28.043
4700	695.253	1916.729	1332.410	2746.302	232.438	2518.161	-27.986
4800	695.713	1931.371	1344.736	2815.850	229.075	2566.860	-27.933
4900	696.146	1945.721	1356.855	2885.443	225.450	2615.548	-27.882
5000	696.555	1959.789	1368.773	2955.079	221.624	2664.434	-27.835

3.34. 1*H*-Benzo[*b*]fluorene



Other names: 2,3-Benzofluorene
Isonaphthofluorene

Formula: C₁₇H₁₂
Mass: 216.277 g/mol

CAS Number: 243-17-4

Point Group: C_s

Length: 13.72 Å
Width: 7.751 Å
Breadth: 4.176 Å
L/B Ratio: 1.770

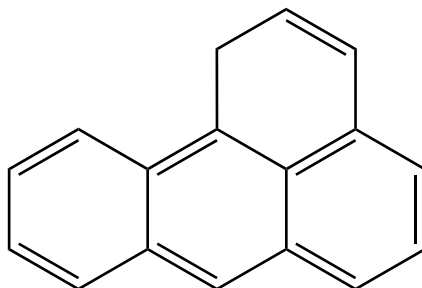
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C	-0.4092	0.2520	0.0000	C	-2.4584	-0.8682	0.0000	H	3.7920	-2.1647	0.0000
C	-0.1227	-1.1568	0.0000	C	-1.8614	0.4144	0.0000	H	5.6413	-0.5053	0.0000
C	1.1612	-1.6105	0.0000	C	-2.6389	1.5597	0.0000	H	5.1449	1.9233	-0.0000
C	0.5915	1.1793	0.0000	C	-4.0282	1.4156	0.0000	H	2.7924	2.7236	-0.0000
C	1.9430	0.7242	0.0000	C	-4.6155	0.1560	0.0000	H	-2.1743	2.5509	0.0000
C	2.2258	-0.6596	0.0000	C	-3.8337	-1.0028	0.0000	H	-4.6611	2.3091	0.0000
C	3.5784	-1.0898	0.0000	H	-1.4869	-2.5936	0.8883	H	-5.7068	0.0668	0.0000
C	4.5976	-0.1744	0.0000	H	-1.4869	-2.5936	-0.8883	H	-4.3010	-1.9923	-0.0000
C	4.3148	1.2094	0.0000	H	1.3917	-2.6812	0.0000				

Table 3.34: Table of thermodynamic data as a function of temperature for 1*H*-Benzo[*b*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-33.691	255.078	255.078	∞
100	75.361	302.386	588.816	-28.643	276.090	307.906	-160.830
200	142.757	374.028	463.645	-17.923	265.104	344.071	-89.860
250	183.179	410.178	449.321	-9.786	259.833	364.423	-76.141
298.15	223.284	445.871	445.871	0.000	255.078	385.009	-67.451
300	224.816	447.257	445.875	0.414	254.903	385.814	-67.175
350	265.285	484.979	448.762	12.676	250.463	407.993	-60.888
400	303.048	522.903	455.660	26.897	246.559	430.764	-56.251
450	337.397	560.615	465.230	42.923	243.143	453.998	-52.698
500	368.201	597.788	476.633	60.578	240.159	477.603	-49.894
600	420.103	669.690	502.868	100.093	235.274	525.574	-45.754
700	461.453	737.671	531.604	144.247	231.659	574.264	-42.851
800	494.881	801.548	561.397	192.121	229.158	623.384	-40.702
900	522.332	861.473	591.445	243.025	227.623	672.754	-39.045
1000	545.163	917.723	621.290	296.434	226.917	722.258	-37.726
1100	564.335	970.608	650.666	351.936	226.887	771.805	-36.649
1200	580.558	1020.426	679.424	409.202	227.419	821.317	-35.750
1300	594.372	1067.456	707.481	467.967	228.374	870.775	-34.987
1400	606.201	1111.947	734.797	528.011	229.654	920.149	-34.330
1500	616.382	1154.127	761.358	589.152	231.190	969.422	-33.758
1600	625.189	1194.195	787.169	651.241	232.888	1018.582	-33.253
1700	632.842	1232.332	812.243	714.152	234.690	1067.615	-32.803
1800	639.524	1268.697	836.599	777.777	236.543	1116.583	-32.402
1900	645.383	1303.435	860.262	842.029	238.419	1165.414	-32.039
2000	650.543	1336.673	883.258	906.831	240.278	1214.162	-31.710
2100	655.105	1368.526	905.612	972.118	242.066	1262.809	-31.410
2200	659.155	1399.096	927.353	1037.835	243.780	1311.377	-31.135
2300	662.763	1428.478	948.507	1103.934	245.412	1359.865	-30.883
2400	665.990	1456.755	969.098	1170.375	246.917	1408.256	-30.649
2500	668.884	1484.001	989.153	1237.121	248.298	1456.660	-30.435
2600	671.490	1510.287	1008.694	1304.142	249.531	1504.936	-30.234
2700	673.843	1535.674	1027.744	1371.411	250.618	1553.211	-30.048
2800	675.974	1560.219	1046.325	1438.903	251.540	1601.467	-29.875
2900	677.909	1583.975	1064.458	1506.599	252.278	1649.656	-29.713
3000	679.671	1606.987	1082.160	1574.479	252.858	1697.839	-29.561
3100	681.279	1629.300	1099.452	1642.528	253.231	1745.959	-29.419
3200	682.751	1650.953	1116.350	1710.730	253.422	1794.116	-29.285
3300	684.102	1671.983	1132.870	1779.074	253.417	1842.293	-29.160
3400	685.343	1692.425	1149.028	1847.547	253.201	1890.422	-29.042
3500	686.487	1712.308	1164.839	1916.139	252.775	1938.547	-28.931
3600	687.542	1731.662	1180.317	1984.842	252.151	1986.740	-28.826
3700	688.519	1750.513	1195.474	2053.645	251.310	2034.969	-28.728
3800	689.424	1768.887	1210.323	2122.543	250.234	2083.180	-28.635
3900	690.264	1786.806	1224.876	2191.528	248.950	2131.394	-28.546
4000	691.045	1804.292	1239.143	2260.594	247.446	2179.730	-28.464
4100	691.772	1821.365	1253.137	2329.735	245.699	2228.059	-28.385
4200	692.451	1838.043	1266.865	2398.947	243.728	2276.427	-28.311
4300	693.085	1854.344	1280.339	2468.224	241.521	2324.789	-28.240
4400	693.678	1870.285	1293.566	2537.562	239.086	2373.264	-28.174
4500	694.234	1885.880	1306.556	2606.958	236.431	2421.834	-28.111
4600	694.755	1901.144	1319.316	2676.408	233.524	2470.466	-28.052
4700	695.245	1916.091	1331.855	2745.908	230.372	2519.094	-27.996
4800	695.705	1930.733	1344.180	2815.456	227.008	2567.857	-27.943
4900	696.139	1945.083	1356.297	2885.048	223.382	2616.608	-27.893
5000	696.547	1959.151	1368.214	2954.683	219.556	2665.558	-27.846

3.35. 1*H*-Benz[*de*]anthracene



Other names: Benzanthrene
H-meso-Benzanthrene

Formula: C₁₇H₁₂

Mass: 216.277 g/mol

CAS Number: 199-95-1

Point Group: C_s

Length: 11.69 Å

Width: 9.172 Å

Breadth: 4.175 Å

L/B Ratio: 1.274

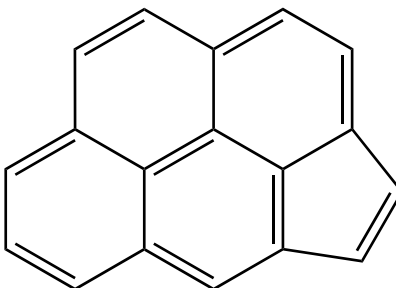
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C	2.9587	1.5065	0.0000	C	-1.0078	0.0055	0.0000	H	-1.6892	3.3840	0.0000
C	2.5373	-1.2603	0.0000	C	-2.3699	-0.4606	0.0000	H	-4.0176	2.5135	0.0000
C	1.3915	-0.3979	0.0000	C	-2.6133	-1.8939	0.0000	H	-4.4468	0.0761	0.0000
C	1.6154	1.0063	0.0000	C	-1.6030	-2.7693	0.0000	H	-3.6574	-2.2279	0.0000
C	0.5348	1.8909	0.0000	C	-0.1767	-2.3644	0.0000	H	-1.7941	-3.8485	0.0000
C	-0.7736	1.4074	0.0000	H	4.6691	-1.4193	0.0000	H	0.3132	-2.8181	0.8881
C	-1.8887	2.3065	0.0000	H	5.0447	1.0293	0.0000	H	0.3132	-2.8181	-0.8881
C	-3.1628	1.8292	0.0000	H	3.1096	2.5922	0.0000				

Table 3.35: Table of thermodynamic data as a function of temperature for 1*H*-Benz[*de*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-33.683	300.002	300.002	∞
100	74.330	299.336	586.816	-28.748	320.909	353.030	-184.400
200	143.636	370.909	461.043	-18.027	309.924	389.516	-101.729
250	184.287	407.288	446.638	-9.837	304.705	410.018	-85.667
298.15	224.287	443.171	443.171	0.000	300.002	430.738	-75.462
300	225.812	444.563	443.175	0.416	299.828	431.548	-75.138
350	266.046	482.421	446.073	12.722	295.433	453.858	-67.733
400	303.571	520.431	452.993	26.975	291.560	476.755	-62.256
450	337.723	558.193	462.587	43.022	288.165	500.111	-58.050
500	368.380	595.392	474.014	60.689	285.194	523.836	-54.724
600	420.118	667.309	500.288	100.213	280.318	572.046	-49.800
700	461.412	735.288	529.052	144.365	276.701	620.974	-46.337
800	494.837	799.159	558.866	192.234	274.195	670.332	-43.767
900	522.304	859.079	588.930	243.134	272.656	719.942	-41.783
1000	545.155	915.328	618.786	296.541	271.948	769.686	-40.203
1100	564.347	968.213	648.173	352.044	271.919	819.472	-38.913
1200	580.584	1018.033	676.939	409.313	272.452	869.224	-37.836
1300	594.409	1065.065	705.003	468.080	273.411	918.920	-36.922
1400	606.246	1109.560	732.325	528.128	274.695	968.533	-36.136
1500	616.432	1151.742	758.892	589.275	276.236	1018.045	-35.451
1600	625.242	1191.814	784.708	651.369	277.939	1067.443	-34.848
1700	632.897	1229.954	809.786	714.285	279.746	1116.715	-34.312
1800	639.579	1266.323	834.147	777.916	281.605	1165.920	-33.833
1900	645.437	1301.063	857.814	842.173	283.487	1214.988	-33.402
2000	650.596	1334.304	880.814	906.980	285.351	1263.973	-33.011
2100	655.157	1366.159	903.172	972.272	287.144	1312.858	-32.655
2200	659.205	1396.732	924.917	1037.994	288.863	1361.662	-32.329
2300	662.811	1426.116	946.073	1104.098	290.500	1410.386	-32.030
2400	666.035	1454.394	966.668	1170.544	292.009	1459.013	-31.754
2500	668.928	1481.643	986.725	1237.294	293.395	1507.653	-31.500
2600	671.532	1507.930	1006.269	1304.320	294.632	1556.164	-31.263
2700	673.883	1533.319	1025.322	1371.592	295.723	1604.675	-31.044
2800	676.012	1557.866	1043.905	1439.089	296.650	1653.166	-30.840
2900	677.945	1581.622	1062.040	1506.788	297.391	1701.591	-30.648
3000	679.705	1604.636	1079.745	1574.672	297.975	1750.009	-30.470
3100	681.312	1626.950	1097.039	1642.724	298.351	1798.364	-30.302
3200	682.783	1648.604	1113.938	1710.930	298.545	1846.756	-30.145
3300	684.132	1669.635	1130.461	1779.277	298.544	1895.168	-29.997
3400	685.372	1690.077	1146.621	1847.753	298.331	1943.532	-29.858
3500	686.514	1709.961	1162.433	1916.348	297.907	1991.892	-29.727
3600	687.569	1729.316	1177.913	1985.053	297.286	2040.319	-29.604
3700	688.544	1748.168	1193.071	2053.859	296.448	2088.783	-29.488
3800	689.448	1766.543	1207.922	2122.759	295.374	2137.228	-29.378
3900	690.287	1784.462	1222.476	2191.746	294.092	2185.677	-29.273
4000	691.067	1801.949	1236.745	2260.815	292.591	2234.247	-29.176
4100	691.794	1819.022	1250.740	2329.958	290.846	2282.810	-29.083
4200	692.472	1835.701	1264.470	2399.172	288.877	2331.413	-28.995
4300	693.105	1852.003	1277.944	2468.451	286.672	2380.008	-28.911
4400	693.697	1867.944	1291.173	2537.791	284.239	2428.717	-28.832
4500	694.252	1883.539	1304.164	2607.189	281.586	2477.522	-28.758
4600	694.773	1898.804	1316.926	2676.641	278.681	2526.388	-28.687
4700	695.262	1913.751	1329.465	2746.143	275.531	2575.249	-28.620
4800	695.721	1928.394	1341.791	2815.692	272.168	2624.246	-28.557
4900	696.154	1942.743	1353.910	2885.286	268.544	2673.232	-28.496
5000	696.562	1956.812	1365.827	2954.922	264.719	2722.415	-28.440

3.36. Cyclopenta[*cd*]pyrene



Other names: Acepyrene
Acepyrylene
3,4-Dihydrocyclopenta[*cd*]pyrene

Formula: C₁₈H₁₀
Mass: 226.272 g/mol
CAS Number: 25732-74-5
Point Group: C_s

Length: 11.47 Å
Width: 9.554 Å
Breadth: 3.884 Å
L/B Ratio: 1.201

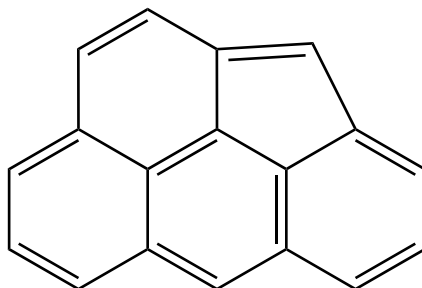
Cartesian coordinates:

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C	-3.4929	1.0242	0.0000	C	-1.7357	-2.4184	0.0000	H	4.3621	-0.7343	0.0000
C	-1.2778	1.7235	0.0000	C	1.0562	0.0930	0.0000	H	4.5398	1.7366	0.0000
C	-0.0644	2.3289	0.0000	C	-0.2209	-0.5392	0.0000	H	2.5261	3.1685	0.0000
C	1.1387	1.5095	0.0000	C	-0.4182	-1.9361	0.0000	H	-3.8603	-1.9865	0.0000
C	3.4548	-0.1200	0.0000	C	0.7785	-2.7415	0.0000	H	-1.8983	-3.5022	0.0000
C	3.5494	1.2683	0.0000	C	2.0085	-2.1666	0.0000	H	0.6666	-3.8314	0.0000
C	2.4166	2.0780	0.0000	C	2.1983	-0.7324	0.0000	H	2.9106	-2.7896	0.0000
C	-1.3314	0.2801	0.0000	H	-3.0185	3.1712	0.0000				
C	-2.6558	-0.1893	0.0000	H	-4.5808	1.0007	0.0000				

Table 3.36: Table of thermodynamic data as a function of temperature for Cyclopenta[*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	–32.128	353.645	353.645	∞
100	66.984	293.194	569.215	–27.602	371.221	393.979	–205.789
200	137.894	359.929	447.774	–17.569	361.917	420.438	–109.805
250	179.722	395.160	433.703	–9.636	357.542	435.575	–91.006
298.15	220.390	430.303	430.303	0.000	353.645	450.967	–79.006
300	221.931	431.671	430.307	0.409	353.502	451.569	–78.624
350	262.394	468.953	433.159	12.528	349.897	468.207	–69.875
400	299.825	506.473	439.979	26.598	346.746	485.323	–63.375
450	333.670	543.777	449.443	42.450	343.990	502.813	–58.364
500	363.880	580.527	460.720	59.904	341.569	520.606	–54.386
600	414.455	651.526	486.656	98.922	337.538	556.810	–48.474
700	454.378	718.530	515.044	142.440	334.453	593.616	–44.295
800	486.344	781.367	544.450	189.533	332.203	630.796	–41.186
900	512.356	840.202	574.079	239.511	330.681	668.208	–38.781
1000	533.815	895.330	603.477	291.853	329.789	705.764	–36.865
1100	551.713	947.073	632.386	346.156	329.404	743.391	–35.300
1200	566.773	995.742	660.658	402.101	329.442	781.021	–33.996
1300	579.539	1041.626	688.215	459.434	329.788	818.642	–32.893
1400	590.430	1084.984	715.022	517.947	330.360	856.230	–31.946
1500	599.775	1126.046	741.067	577.469	331.110	893.772	–31.123
1600	607.839	1165.018	766.356	637.859	331.956	931.255	–30.402
1700	614.833	1202.083	790.906	699.001	332.851	968.667	–29.763
1800	620.928	1237.402	814.738	760.796	333.750	1006.068	–29.195
1900	626.266	1271.120	837.877	823.161	334.634	1043.385	–28.684
2000	630.960	1303.365	860.352	886.028	335.468	1080.673	–28.224
2100	635.107	1334.252	882.188	949.335	336.204	1117.913	–27.806
2200	638.784	1363.884	903.414	1013.033	336.841	1155.122	–27.426
2300	642.058	1392.353	924.058	1077.079	337.377	1192.303	–27.078
2400	644.984	1419.742	944.144	1141.433	337.767	1229.433	–26.757
2500	647.607	1446.125	963.699	1206.065	338.019	1266.623	–26.464
2600	649.968	1471.572	982.746	1270.946	338.110	1303.730	–26.192
2700	652.098	1496.142	1001.309	1336.051	338.043	1340.884	–25.940
2800	654.026	1519.893	1019.408	1401.359	337.801	1378.057	–25.707
2900	655.777	1542.875	1037.064	1466.850	337.367	1415.208	–25.490
3000	657.370	1565.134	1054.297	1532.509	336.769	1452.394	–25.288
3100	658.825	1586.713	1071.126	1598.320	335.955	1489.553	–25.098
3200	660.155	1607.651	1087.567	1664.270	334.955	1526.789	–24.922
3300	661.376	1627.984	1103.636	1730.347	333.757	1564.086	–24.757
3400	662.497	1647.745	1119.350	1796.542	332.341	1601.364	–24.601
3500	663.530	1666.964	1134.723	1862.844	330.712	1638.675	–24.455
3600	664.484	1685.670	1149.769	1929.245	328.885	1676.095	–24.319
3700	665.366	1703.888	1164.500	1995.738	326.838	1713.578	–24.191
3800	666.183	1721.644	1178.929	2062.316	324.555	1751.080	–24.070
3900	666.941	1738.958	1193.067	2128.973	322.062	1788.611	–23.955
4000	667.646	1755.852	1206.927	2195.703	319.350	1826.301	–23.849
4100	668.303	1772.346	1220.517	2262.500	316.395	1864.012	–23.747
4200	668.915	1788.458	1233.848	2329.362	313.215	1901.792	–23.652
4300	669.487	1804.205	1246.930	2396.282	309.802	1939.592	–23.561
4400	670.022	1819.602	1259.771	2463.258	306.160	1977.534	–23.476
4500	670.523	1834.665	1272.380	2530.285	302.301	2015.598	–23.396
4600	670.994	1849.408	1284.764	2597.362	298.189	2053.756	–23.321
4700	671.435	1863.843	1296.932	2664.483	293.835	2091.931	–23.249
4800	671.851	1877.984	1308.890	2731.648	289.268	2130.271	–23.182
4900	672.242	1891.841	1320.646	2798.853	284.441	2168.619	–23.117
5000	672.610	1905.426	1332.207	2866.095	279.415	2207.191	–23.058

3.37. Benz[*mno*]aceanthrylene



Other names: Naphtho[1,8,7,6-*cdef*]fluorene

Formula: C₁₈H₁₀

Mass: 226.272 g/mol

CAS Number: 203-13-4

Point Group: C_s

Length: 11.85 Å

Width: 9.674 Å

Breadth: 3.884 Å

L/B Ratio: 1.225

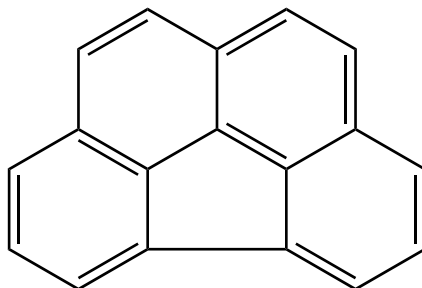
Cartesian coordinates:

C	-2.2473	2.0661	0.0000	C	1.2713	-0.0123	0.0000	H	4.8430	-1.1767	0.0000
C	-2.3599	0.6058	0.0000	C	1.4289	-1.4004	0.0000	H	4.4247	1.2499	0.0000
C	-1.1360	-0.1338	0.0000	C	0.2469	-2.1667	0.0000	H	0.3098	-3.2606	0.0000
C	0.0279	0.5975	0.0000	C	2.8086	-1.7997	0.0000	H	-4.4986	0.3631	0.0000
C	0.1898	2.0427	0.0000	C	3.7967	-0.8496	0.0000	H	-4.4028	-2.1004	0.0000
C	-1.0738	2.7497	0.0000	C	3.5668	0.5708	0.0000	H	-2.2704	-3.3421	0.0000
C	-1.0252	-1.5507	0.0000	C	2.2788	1.0156	0.0000	H	-1.0603	3.8443	0.0000
C	-2.2757	-2.2466	0.0000	C	1.5399	2.3066	0.0000	H	-3.1957	2.6165	0.0000
C	-3.4543	-1.5514	0.0000	H	2.0290	3.2774	0.0000				
C	-3.5190	-0.1264	0.0000	H	3.0541	-2.8668	0.0000				

Table 3.37: Table of thermodynamic data as a function of temperature for Benz[*mno*]aceanthrylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-32.302	430.636	430.636	∞
100	67.232	294.220	571.643	-27.742	448.072	470.727	-245.878
200	138.645	361.270	449.574	-17.661	438.816	497.069	-129.818
250	180.679	396.694	435.431	-9.684	434.484	512.134	-107.002
298.15	221.434	432.014	432.014	0.000	430.636	527.448	-92.405
300	222.976	433.388	432.018	0.411	430.495	528.047	-91.939
350	263.436	470.832	434.883	12.582	426.943	544.595	-81.275
400	300.812	508.488	441.730	26.703	423.842	561.613	-73.338
450	334.578	545.904	451.230	42.603	421.133	579.000	-67.207
500	364.702	582.745	462.546	60.100	418.756	596.684	-62.334
600	415.123	653.880	488.559	99.192	414.800	632.659	-55.077
700	454.924	720.977	517.019	142.771	411.774	669.225	-49.937
800	486.799	783.881	546.489	189.914	409.574	706.156	-46.106
900	512.742	842.765	576.173	239.933	408.094	743.315	-43.140
1000	534.148	897.931	605.620	292.311	407.238	780.612	-40.774
1100	552.005	949.703	634.571	346.645	406.884	817.977	-38.842
1200	567.031	998.397	662.882	402.618	406.949	855.343	-37.231
1300	579.769	1044.300	690.473	459.975	407.319	892.698	-35.868
1400	590.636	1087.674	717.310	518.509	407.914	930.018	-34.699
1500	599.962	1128.749	743.382	578.051	408.683	967.290	-33.683
1600	608.008	1167.733	768.696	638.459	409.547	1004.502	-32.793
1700	614.987	1204.808	793.268	699.617	410.458	1041.642	-32.005
1800	621.069	1240.135	817.121	761.427	411.372	1078.770	-31.304
1900	626.395	1273.861	840.279	823.806	412.269	1115.813	-30.675
2000	631.079	1306.112	862.770	886.684	413.116	1152.827	-30.108
2100	635.216	1337.005	884.622	950.003	413.863	1189.792	-29.594
2200	638.885	1366.641	905.863	1013.712	414.510	1226.725	-29.126
2300	642.152	1395.114	926.520	1077.767	415.056	1263.631	-28.697
2400	645.071	1422.507	946.619	1142.131	415.455	1300.484	-28.304
2500	647.689	1448.894	966.186	1206.771	415.715	1337.398	-27.943
2600	650.044	1474.344	985.244	1271.660	415.814	1374.227	-27.608
2700	652.169	1498.917	1003.816	1336.772	415.755	1411.104	-27.299
2800	654.093	1522.670	1021.925	1402.087	415.520	1448.000	-27.012
2900	655.839	1545.654	1039.590	1467.585	415.092	1484.873	-26.745
3000	657.429	1567.915	1056.832	1533.249	414.500	1521.781	-26.496
3100	658.880	1589.496	1073.669	1599.066	413.692	1558.661	-26.263
3200	660.208	1610.436	1090.117	1665.021	412.698	1595.619	-26.045
3300	661.425	1630.771	1106.194	1731.104	411.504	1632.637	-25.842
3400	662.544	1650.533	1121.915	1797.303	410.093	1669.637	-25.650
3500	663.575	1669.754	1137.294	1863.610	408.469	1706.669	-25.470
3600	664.526	1688.461	1152.345	1930.015	406.646	1743.809	-25.301
3700	665.406	1706.680	1167.082	1996.512	404.603	1781.013	-25.143
3800	666.221	1724.436	1181.517	2063.094	402.324	1818.237	-24.993
3900	666.977	1741.752	1195.661	2129.755	399.835	1855.488	-24.851
4000	667.681	1758.647	1209.525	2196.488	397.126	1892.898	-24.718
4100	668.336	1775.142	1223.120	2263.289	394.175	1930.330	-24.592
4200	668.946	1791.255	1236.456	2330.154	390.998	1967.831	-24.473
4300	669.517	1807.002	1249.542	2397.077	387.588	2005.351	-24.360
4400	670.051	1822.400	1262.387	2464.056	383.949	2043.013	-24.253
4500	670.551	1837.464	1275.000	2531.086	380.093	2080.797	-24.153
4600	671.020	1852.207	1287.388	2598.165	375.983	2118.676	-24.058
4700	671.461	1866.643	1299.560	2665.289	371.632	2156.571	-23.967
4800	671.875	1880.784	1311.522	2732.456	367.068	2194.631	-23.882
4900	672.265	1894.641	1323.281	2799.664	362.243	2232.699	-23.800
5000	672.633	1908.227	1334.845	2866.909	357.219	2270.991	-23.724

3.38. Benzo[ghi]fluoranthene



Other names: Benzo[*mno*]fluoranthene
2,13-Benzofluoranthene
7,10-Benzofluoranthene
Benzofluoranthene

Formula: C₁₈H₁₀
Mass: 226.272 g/mol
CAS Number: 203-12-3
Point Group: C_{2v}

Length: 11.38 Å
Width: 9.630 Å
Breadth: 3.884 Å
L/B Ratio: 1.182

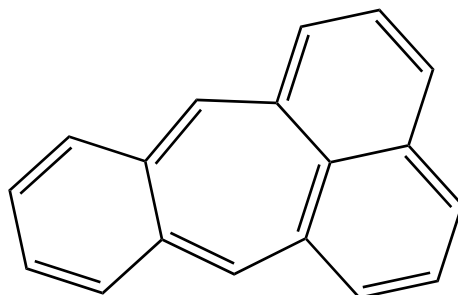
Cartesian coordinates:

C	-0.7491	-1.4850	0.0000	C	2.4558	1.8763	0.0000	H	-1.6224	-3.4617	0.0000
C	-3.4440	-0.5275	0.0000	C	1.3275	2.6661	0.0000	H	-1.4082	3.7629	0.0000
C	-3.1185	-1.8697	0.0000	C	2.4089	0.4345	0.0000	H	-3.4351	2.3621	0.0000
C	-1.7861	-2.3801	0.0000	C	1.1388	-0.1089	0.0000	H	3.4449	2.3478	0.0000
C	-2.4070	0.4445	0.0000	C	0.7429	-1.4881	0.0000	H	1.4239	3.7570	0.0000
C	-1.1393	-0.1042	0.0000	C	1.7762	-2.3875	0.0000	H	1.6080	-3.4684	0.0000
C	-1.3164	2.6716	0.0000	C	3.1107	-1.8826	0.0000	H	3.9211	-2.6208	0.0000
C	-2.4480	1.8865	0.0000	C	3.4418	-0.5418	0.0000	H	4.4893	-0.2242	0.0000
C	0.0044	2.0987	0.0000	H	-4.4902	-0.2056	0.0000				
C	0.0015	0.7270	0.0000	H	-3.9320	-2.6045	0.0000				

Table 3.38: Table of thermodynamic data as a function of temperature for Benzo[ghi]fluoranthene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-32.087	375.174	375.174	∞
100	67.480	289.506	564.247	-27.474	392.878	416.004	-217.294
200	137.093	356.134	443.454	-17.464	383.550	442.830	-115.653
250	178.622	391.152	429.468	-9.579	379.127	458.162	-95.726
298.15	219.155	426.088	426.088	0.000	375.174	473.752	-82.998
300	220.693	427.448	426.092	0.407	375.028	474.363	-82.592
350	261.118	464.535	428.928	12.462	371.360	491.216	-73.309
400	298.568	501.885	435.713	26.469	368.145	508.557	-66.409
450	332.466	539.044	445.134	42.260	365.328	526.281	-61.088
500	362.746	575.671	456.362	59.655	362.849	544.313	-56.863
600	413.486	646.477	482.198	98.568	358.713	581.013	-50.581
700	453.572	713.345	510.492	141.997	355.538	618.331	-46.140
800	485.686	776.084	539.812	189.017	353.215	656.034	-42.834
900	511.821	834.849	569.365	238.936	351.634	693.979	-40.277
1000	533.382	889.926	598.697	291.229	350.693	732.073	-38.239
1100	551.362	941.631	627.547	345.493	350.270	770.242	-36.575
1200	566.488	990.273	655.767	401.407	350.276	808.418	-35.189
1300	579.305	1036.136	683.279	458.714	350.596	846.587	-34.016
1400	590.236	1079.478	710.046	517.205	351.147	884.725	-33.009
1500	599.615	1120.528	736.055	576.709	351.879	922.818	-32.135
1600	607.705	1159.491	761.313	637.085	352.710	960.853	-31.368
1700	614.719	1196.548	785.834	698.215	353.593	998.818	-30.689
1800	620.832	1231.861	809.640	759.999	354.482	1036.773	-30.086
1900	626.183	1265.575	832.756	822.356	355.356	1074.644	-29.543
2000	630.889	1297.816	855.209	885.214	356.183	1112.487	-29.055
2100	635.045	1328.700	877.026	948.515	356.912	1150.282	-28.611
2200	638.730	1358.329	898.234	1012.208	357.543	1188.046	-28.207
2300	642.011	1386.795	918.861	1076.248	358.075	1225.784	-27.838
2400	644.942	1414.182	938.933	1140.598	358.460	1263.469	-27.498
2500	647.570	1440.564	958.474	1205.226	358.708	1301.215	-27.187
2600	649.935	1466.009	977.508	1270.103	358.795	1338.878	-26.898
2700	652.068	1490.578	996.058	1335.205	358.725	1376.589	-26.631
2800	653.999	1514.328	1014.146	1400.510	358.481	1414.319	-26.384
2900	655.753	1537.309	1031.792	1465.999	358.044	1452.026	-26.153
3000	657.348	1559.567	1049.015	1531.656	357.443	1489.769	-25.939
3100	658.805	1581.146	1065.835	1597.464	356.628	1527.484	-25.737
3200	660.137	1602.083	1082.267	1663.412	355.626	1565.277	-25.550
3300	661.359	1622.416	1098.328	1729.488	354.426	1603.130	-25.375
3400	662.482	1642.176	1114.035	1795.681	353.009	1640.966	-25.210
3500	663.516	1661.395	1129.400	1861.981	351.378	1678.834	-25.055
3600	664.471	1680.100	1144.439	1928.381	349.549	1716.810	-24.910
3700	665.354	1698.318	1159.163	1994.873	347.501	1754.850	-24.774
3800	666.171	1716.073	1173.586	2061.450	345.217	1792.910	-24.645
3900	666.930	1733.387	1187.719	2128.106	342.723	1830.997	-24.523
4000	667.636	1750.281	1201.573	2194.834	340.010	1869.244	-24.409
4100	668.293	1766.775	1215.158	2261.631	337.054	1907.512	-24.302
4200	668.906	1782.887	1228.484	2328.492	333.873	1945.850	-24.200
4300	669.479	1798.634	1241.561	2395.411	330.459	1984.207	-24.103
4400	670.015	1814.031	1254.398	2462.386	326.817	2022.706	-24.012
4500	670.516	1829.094	1267.002	2529.413	322.957	2061.327	-23.927
4600	670.987	1843.836	1279.382	2596.488	318.844	2100.043	-23.846
4700	671.429	1858.271	1291.546	2663.609	314.489	2138.775	-23.769
4800	671.845	1872.411	1303.500	2730.773	309.922	2177.672	-23.697
4900	672.236	1886.268	1315.253	2797.977	305.094	2216.577	-23.629
5000	672.605	1899.853	1326.809	2865.220	300.067	2255.707	-23.565

3.39. Pleiadene



Other names: Benzo[5,6]cyclohepta[1,2,3-*de*]naphthalene
Benzopleiadiene

Formula: C₁₈H₁₂
Mass: 228.29 g/mol

CAS Number: 206-92-8

Point Group: C_{2v}

Length: 12.34 Å

Width: 9.239 Å

Breadth: 3.897 Å

L/B Ratio: 1.336

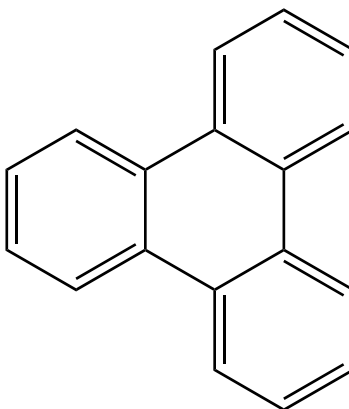
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C	0.0309	1.4692	0.0066	C	-2.4887	-0.5898	0.0207	H	3.4420	2.0417	-0.0170
C	0.0510	-0.0014	0.0004	C	-3.2524	-1.7679	0.0265	H	3.4768	-0.4794	-0.0291
C	-1.0544	-0.8154	0.0067	C	-4.6551	-1.7641	0.0371	H	1.3660	-1.7451	-0.0185
C	1.3146	2.1555	0.0001	C	-5.3281	-0.5649	0.0407	H	-0.8850	3.3265	0.0194
C	2.4992	1.4901	-0.0122	C	-4.6190	0.6703	0.0362	H	-2.7247	-2.7239	0.0222
C	2.5190	0.0457	-0.0192	C	-5.3615	1.8858	0.0410	H	-5.2014	-2.7103	0.0422
C	1.3532	-0.6522	-0.0133	C	-4.7213	3.1030	0.0401	H	-6.4203	-0.5356	0.0485
C	-1.0964	2.2526	0.0172	C	-3.3193	3.1447	0.0334	H	-6.4525	1.8272	0.0456
C	-2.5239	1.9878	0.0260	H	-0.8147	-1.8834	0.0001	H	-5.2933	4.0338	0.0448
C	-3.1740	0.6899	0.0272	H	1.2980	3.2485	0.0054	H	-2.8174	4.1146	0.0331

Table 3.39: Table of thermodynamic data as a function of temperature for Pleiadene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-35.486	424.656	424.656	∞
100	77.959	301.850	604.933	-30.308	444.993	476.958	-249.132
200	151.571	377.230	472.296	-19.013	434.256	513.200	-134.031
250	194.418	415.619	457.105	-10.372	429.194	533.522	-111.471
298.15	236.297	453.450	453.450	0.000	424.656	554.038	-97.063
300	237.888	454.917	453.455	0.439	424.488	554.840	-96.604
350	279.766	494.764	456.506	13.390	420.268	576.907	-86.097
400	318.663	534.698	463.786	28.365	416.565	599.537	-78.290
450	353.958	574.306	473.870	45.196	413.326	622.606	-72.269
500	385.569	613.267	485.868	63.699	410.493	646.029	-67.489
600	438.776	688.456	513.422	105.020	405.835	693.596	-60.382
700	481.116	759.393	543.547	151.093	402.366	741.850	-55.356
800	515.310	825.948	574.732	200.972	399.950	790.517	-51.614
900	543.366	888.315	606.147	253.951	398.454	839.427	-48.718
1000	566.684	946.808	637.319	309.488	397.754	888.468	-46.408
1100	586.258	1001.763	667.978	367.163	397.703	937.553	-44.520
1200	602.816	1053.504	697.971	426.639	398.193	986.606	-42.945
1300	616.915	1102.326	727.215	487.644	399.090	1035.609	-41.610
1400	628.987	1148.498	755.673	549.955	400.296	1084.533	-40.464
1500	639.378	1192.256	783.332	613.386	401.748	1133.363	-39.466
1600	648.368	1233.815	810.200	677.784	403.349	1182.084	-38.590
1700	656.180	1273.362	836.291	743.020	405.046	1230.685	-37.814
1800	663.002	1311.065	861.628	808.987	406.783	1279.229	-37.121
1900	668.984	1347.076	886.238	875.593	408.534	1327.641	-36.499
2000	674.253	1381.527	910.147	942.760	410.260	1375.978	-35.936
2100	678.912	1414.539	933.385	1010.423	411.905	1424.220	-35.425
2200	683.048	1446.219	955.981	1078.525	413.467	1472.390	-34.958
2300	686.734	1476.665	977.962	1147.018	414.939	1520.487	-34.531
2400	690.030	1505.963	999.355	1215.859	416.275	1568.493	-34.137
2500	692.987	1534.192	1020.187	1285.012	417.478	1616.522	-33.775
2600	695.649	1561.425	1040.484	1354.447	418.524	1664.427	-33.438
2700	698.053	1587.724	1060.268	1424.134	419.415	1712.341	-33.127
2800	700.230	1613.151	1079.562	1494.050	420.133	1760.244	-32.837
2900	702.208	1637.758	1098.388	1564.173	420.657	1808.086	-32.566
3000	704.008	1661.595	1116.766	1634.485	421.015	1855.930	-32.314
3100	705.652	1684.706	1134.716	1704.970	421.155	1903.717	-32.077
3200	707.157	1707.134	1152.255	1775.611	421.105	1951.550	-31.855
3300	708.537	1728.916	1169.402	1846.397	420.850	1999.413	-31.647
3400	709.806	1750.087	1186.171	1917.315	420.374	2047.231	-31.451
3500	710.975	1770.679	1202.578	1988.355	419.678	2095.053	-31.266
3600	712.054	1790.724	1218.638	2059.507	418.776	2142.955	-31.093
3700	713.052	1810.247	1234.365	2130.763	417.648	2190.900	-30.929
3800	713.977	1829.275	1249.771	2202.115	416.274	2238.833	-30.774
3900	714.836	1847.832	1264.869	2273.556	414.683	2286.776	-30.627
4000	715.634	1865.941	1279.671	2345.080	412.863	2334.853	-30.489
4100	716.378	1883.621	1294.186	2416.681	410.790	2382.929	-30.358
4200	717.072	1900.892	1308.427	2488.354	408.483	2431.052	-30.234
4300	717.720	1917.773	1322.402	2560.094	405.931	2479.173	-30.115
4400	718.326	1934.280	1336.122	2631.896	403.142	2527.419	-30.004
4500	718.894	1950.429	1349.594	2703.758	400.123	2575.769	-29.898
4600	719.427	1966.236	1362.828	2775.674	396.842	2624.191	-29.798
4700	719.928	1981.713	1375.832	2847.642	393.306	2672.612	-29.702
4800	720.399	1996.875	1388.613	2919.659	389.548	2721.182	-29.612
4900	720.842	2011.734	1401.178	2991.721	385.518	2769.742	-29.525
5000	721.260	2026.301	1413.536	3063.826	381.280	2818.515	-29.444

3.40. Triphenylene



Other names: Benzo[*l*]phenanthrene
9,10-Benzophenanthrene
1,2,3,4-Dibenznaphthalene
Isochrysene

Formula: C₁₈H₁₂
Mass: 228.288 g/mol
CAS Number: 217-59-4
Point Group: D_{3h}

Length: 11.65 Å
Width: 10.41 Å
Breadth: 3.888 Å
L/B Ratio: 1.118

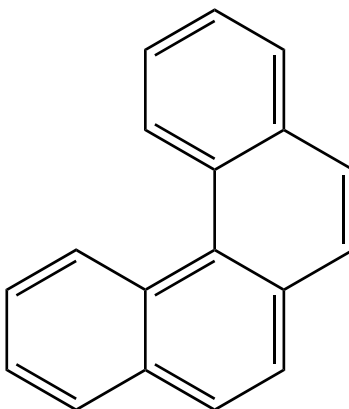
Cartesian coordinates:

C	-1.1563	0.8409	0.0000	C	-1.5591	-3.3952	0.0000	H	-3.0510	3.6851	0.0000
C	0.1216	1.4246	0.0000	C	-0.3042	-2.8203	0.0000	H	-3.2880	1.2083	0.0000
C	0.2348	2.8270	0.0000	C	1.3064	0.5809	0.0000	H	-3.4573	-0.5646	0.0000
C	-0.8887	3.6289	0.0000	C	1.1730	-0.8176	0.0000	H	-3.6930	-3.0414	0.0000
C	-2.1608	3.0479	0.0000	C	2.3308	-1.6169	0.0000	H	-1.6658	-4.4848	0.0000
C	-2.2904	1.6736	0.0000	C	3.5870	-1.0448	0.0000	H	0.5976	-3.4516	0.0000
C	-0.1501	-1.4219	0.0000	C	3.7199	0.3474	0.0000	H	2.2175	-2.7118	0.0000
C	-1.2945	-0.6070	0.0000	C	2.5946	1.1468	0.0000	H	4.4804	-1.6775	0.0000
C	-2.5657	-1.2101	0.0000	H	1.2397	3.2763	0.0000	H	4.7169	0.7997	0.0000
C	-2.6983	-2.5841	0.0000	H	-0.7874	4.7189	0.0000	H	2.6904	2.2433	0.0000

Table 3.40: Table of thermodynamic data as a function of temperature for Triphenylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-35.559	285.004	285.004	∞
100	79.943	299.694	600.314	-30.062	290.684	322.864	-168.644
200	149.884	375.137	469.032	-18.779	279.935	359.297	-93.837
250	191.934	413.052	454.029	-10.244	274.766	379.736	-79.340
298.15	233.558	450.418	450.418	0.000	270.100	400.386	-70.145
300	235.147	451.868	450.423	0.434	269.928	401.194	-69.853
350	277.103	491.295	453.441	13.249	265.571	423.425	-63.191
400	316.233	530.888	460.648	28.096	261.740	446.237	-58.271
450	351.805	570.225	470.642	44.813	258.387	469.504	-54.497
500	383.678	608.973	482.543	63.215	255.453	493.135	-51.516
600	437.289	683.856	509.909	104.368	250.628	541.148	-47.110
700	479.879	754.585	539.862	150.306	247.024	589.873	-44.016
800	514.221	820.984	570.897	200.070	244.492	639.029	-41.723
900	542.369	883.229	602.180	252.944	242.892	688.442	-39.955
1000	565.753	941.620	633.235	308.385	242.095	737.997	-38.548
1100	585.381	996.489	663.789	365.970	241.954	787.605	-37.399
1200	601.989	1048.156	693.688	425.361	242.359	837.190	-36.441
1300	616.135	1096.914	722.848	486.286	243.176	886.730	-35.629
1400	628.254	1143.030	751.229	548.521	244.307	936.198	-34.929
1500	638.690	1186.739	778.819	611.880	245.686	985.578	-34.320
1600	647.722	1228.255	805.622	676.212	247.222	1034.853	-33.784
1700	655.575	1267.763	831.654	741.386	248.856	1084.012	-33.307
1800	662.435	1305.434	856.937	807.294	250.534	1133.117	-32.882
1900	668.454	1341.414	881.496	873.845	252.231	1182.094	-32.497
2000	673.756	1375.839	905.359	940.961	253.905	1230.998	-32.150
2100	678.447	1408.828	928.554	1008.575	255.501	1279.811	-31.833
2200	682.612	1440.487	951.109	1076.632	257.018	1328.552	-31.543
2300	686.324	1470.914	973.052	1145.083	258.449	1377.224	-31.277
2400	689.645	1500.195	994.410	1213.884	259.744	1425.806	-31.031
2500	692.625	1528.409	1015.209	1283.000	260.910	1474.412	-30.806
2600	695.309	1555.628	1035.474	1352.399	261.921	1522.896	-30.595
2700	697.732	1581.915	1055.229	1422.053	262.779	1571.391	-30.400
2800	699.927	1607.330	1074.495	1491.938	263.466	1619.875	-30.219
2900	701.921	1631.927	1093.295	1562.032	263.960	1668.300	-30.049
3000	703.738	1655.754	1111.649	1632.317	264.291	1716.728	-29.890
3100	705.396	1678.857	1129.575	1702.775	264.405	1765.099	-29.741
3200	706.914	1701.277	1147.092	1773.391	264.329	1813.517	-29.602
3300	708.306	1723.051	1164.217	1844.153	264.051	1861.966	-29.472
3400	709.587	1744.216	1180.966	1915.049	263.553	1910.371	-29.349
3500	710.766	1764.802	1197.354	1986.067	262.835	1958.781	-29.233
3600	711.856	1784.841	1213.396	2057.199	261.913	2007.270	-29.124
3700	712.863	1804.359	1229.106	2128.436	260.766	2055.804	-29.022
3800	713.797	1823.382	1244.495	2199.769	259.373	2104.327	-28.925
3900	714.664	1841.934	1259.577	2271.193	257.765	2152.859	-28.834
4000	715.470	1860.038	1274.364	2342.700	255.928	2201.526	-28.748
4100	716.221	1877.715	1288.865	2414.285	253.839	2250.192	-28.667
4200	716.921	1894.982	1303.091	2485.942	251.516	2298.906	-28.590
4300	717.576	1911.860	1317.053	2557.668	248.950	2347.618	-28.517
4400	718.188	1928.363	1330.760	2629.456	246.146	2396.455	-28.449
4500	718.762	1944.510	1344.220	2701.304	243.114	2445.398	-28.385
4600	719.300	1960.313	1357.442	2773.207	239.819	2494.412	-28.324
4700	719.805	1975.788	1370.434	2845.163	236.271	2543.425	-28.266
4800	720.281	1990.947	1383.204	2917.167	232.501	2592.587	-28.213
4900	720.729	2005.804	1395.759	2989.218	228.460	2641.740	-28.161
5000	721.151	2020.369	1408.106	3061.312	224.210	2691.106	-28.113

3.41. Benzo[c]phenanthrene



Other names: 3,4-Benzophenanthrene

Tetrahelicene

Formula: $C_{18}H_{12}$

Mass: 228.288 g/mol

CAS Number: 195-19-7

Point Group: C_2

Length: 12.02 Å

Width: 9.327 Å

Breadth: 4.626 Å

L/B Ratio: 1.289

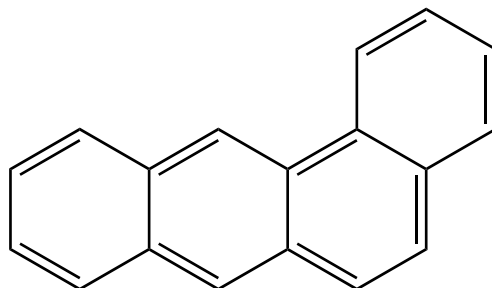
Cartesian coordinates:

C	2.6784	-2.2486	0.4178	C	-1.2093	2.5243	0.1909	H	4.6186	0.4255	-0.3892
C	3.8336	-1.5118	0.1023	C	-2.3957	1.8825	0.3270	H	0.5623	-2.2457	0.6723
C	3.7255	-0.1720	-0.1725	C	-1.2836	-0.2836	-0.0547	H	3.3214	2.4356	-0.5226
C	1.4427	-1.6493	0.3974	C	-2.4609	0.4638	0.1657	H	1.1519	3.6177	-0.2459
C	1.2836	-0.2836	0.0547	C	-3.7255	-0.1720	0.1725	H	-1.1519	3.6177	0.2459
C	2.4609	0.4638	-0.1657	C	-3.8336	-1.5118	-0.1023	H	-3.3214	2.4357	0.5226
C	2.3957	1.8825	-0.3270	C	-2.6784	-2.2486	-0.4178	H	-4.6186	0.4256	0.3892
C	1.2094	2.5243	-0.1909	C	-1.4428	-1.6493	-0.3974	H	-4.8091	-2.0083	-0.0964
C	0.0000	0.3855	-0.0000	H	2.7729	-3.3059	0.6867	H	-2.7730	-3.3059	-0.6867
C	0.0000	1.7854	-0.0000	H	4.8091	-2.0083	0.0963	H	-0.5623	-2.2457	-0.6723

Table 3.41: Table of thermodynamic data as a function of temperature for Benzo[*c*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-34.876	305.237	305.237	∞
100	76.837	298.509	596.432	-29.792	316.154	348.453	-182.009
200	148.642	372.402	466.014	-18.722	305.192	385.101	-100.576
250	191.405	410.121	451.044	-10.231	299.979	405.682	-84.761
298.15	233.497	447.437	447.437	0.000	295.300	426.475	-74.715
300	235.100	448.886	447.442	0.433	295.127	427.288	-74.396
350	277.347	488.330	450.460	13.254	290.776	449.668	-67.108
400	316.639	527.968	457.672	28.118	286.962	472.627	-61.718
450	352.294	567.358	467.675	44.857	283.631	496.039	-57.577
500	384.207	606.160	479.589	63.285	280.723	519.812	-54.303
600	437.838	681.141	506.987	104.493	275.953	568.102	-49.457
700	480.422	751.954	536.976	150.485	272.403	617.094	-46.047
800	514.753	818.426	568.047	200.303	269.925	666.509	-43.518
900	542.887	880.732	599.366	253.230	268.378	716.174	-41.565
1000	566.254	939.177	630.456	308.722	267.632	765.976	-40.010
1100	585.861	994.093	661.043	366.356	267.540	815.826	-38.740
1200	602.446	1045.801	690.973	425.794	267.992	865.648	-37.680
1300	616.568	1094.595	720.162	486.763	268.853	915.423	-36.781
1400	628.662	1140.741	748.570	549.040	270.026	965.121	-36.008
1500	639.073	1184.478	776.185	612.439	271.445	1014.728	-35.335
1600	648.081	1226.017	803.013	676.807	273.017	1064.228	-34.743
1700	655.911	1265.548	829.067	742.016	274.686	1113.610	-34.216
1800	662.750	1303.236	854.371	807.957	276.397	1162.936	-33.747
1900	668.748	1339.234	878.950	874.538	278.124	1212.131	-33.323
2000	674.032	1373.673	902.832	941.683	279.827	1261.253	-32.940
2100	678.704	1406.674	926.044	1009.324	281.450	1310.281	-32.591
2200	682.853	1438.345	948.615	1077.406	282.992	1359.238	-32.272
2300	686.551	1468.783	970.574	1145.880	284.446	1408.123	-31.979
2400	689.857	1498.073	991.947	1214.703	285.763	1456.917	-31.708
2500	692.825	1526.296	1012.760	1283.840	286.950	1505.736	-31.460
2600	695.496	1553.522	1033.038	1353.258	287.980	1554.431	-31.228
2700	697.909	1579.816	1052.805	1422.930	288.856	1603.136	-31.014
2800	700.094	1605.237	1072.083	1492.832	289.560	1651.829	-30.815
2900	702.079	1629.840	1090.894	1562.943	290.071	1700.463	-30.628
3000	703.886	1653.672	1109.258	1633.242	290.416	1749.099	-30.454
3100	705.537	1676.780	1127.195	1703.715	290.545	1797.678	-30.290
3200	707.047	1699.204	1144.721	1774.345	290.483	1846.304	-30.137
3300	708.433	1720.982	1161.855	1845.120	290.218	1894.960	-29.994
3400	709.707	1742.150	1178.613	1916.028	289.732	1943.572	-29.859
3500	710.881	1762.740	1195.009	1987.058	289.026	1992.188	-29.731
3600	711.964	1782.782	1211.059	2058.201	288.115	2040.884	-29.612
3700	712.967	1802.303	1226.776	2129.448	286.978	2089.623	-29.500
3800	713.896	1821.329	1242.173	2200.792	285.596	2138.351	-29.393
3900	714.758	1839.884	1257.262	2272.225	283.997	2187.088	-29.292
4000	715.560	1857.990	1272.055	2343.741	282.169	2235.961	-29.198
4100	716.307	1875.669	1286.562	2415.335	280.089	2284.831	-29.109
4200	717.004	1892.938	1300.795	2487.001	277.775	2333.750	-29.024
4300	717.655	1909.817	1314.763	2558.734	275.216	2382.666	-28.943
4400	718.264	1926.323	1328.475	2630.530	272.420	2431.707	-28.867
4500	718.834	1942.471	1341.941	2702.386	269.396	2480.854	-28.796
4600	719.369	1958.276	1355.168	2774.296	266.108	2530.072	-28.729
4700	719.872	1973.752	1368.165	2846.258	262.566	2579.289	-28.665
4800	720.345	1988.913	1380.940	2918.270	258.804	2628.654	-28.605
4900	720.791	2003.771	1393.500	2990.327	254.769	2678.011	-28.547
5000	721.210	2018.337	1405.852	3062.427	250.525	2727.580	-28.494

3.42. Benz[*a*]anthracene



Other names: 1,2-Benzanthracene
1,2-Benzanthrene
Benzo[*b*]phenanthrene
2,3-Benzophenanthrene
Tetraphene
Naphthanthracene

Formula: C₁₈H₁₂
Mass: 228.288 g/mol
CAS Number: 56-55-3
Point Group: C_s

Length: 13.80 Å
Width: 8.704 Å
Breadth: 3.883 Å
L/B Ratio: 1.585

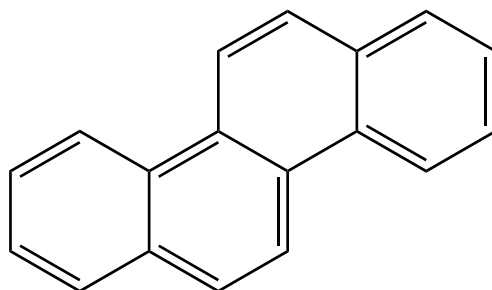
Cartesian coordinates:

C	4.3276	-1.3720	0.0000	C	-0.9585	2.3538	0.0000	H	4.0707	2.0386	0.0000
C	4.7179	-0.0062	0.0000	C	-2.2708	2.0403	0.0000	H	2.6973	-2.7657	0.0000
C	3.7786	0.9824	0.0000	C	-1.7551	-0.3698	0.0000	H	1.7064	2.7132	0.0000
C	3.0077	-1.7148	0.0000	C	-2.7060	0.6648	0.0000	H	0.3218	-2.0907	0.0000
C	1.9997	-0.7038	0.0000	C	-4.0775	0.3501	0.0000	H	-0.6272	3.3988	0.0000
C	2.3883	0.6571	0.0000	C	-4.4898	-0.9671	0.0000	H	-3.0395	2.8217	0.0000
C	1.4013	1.6594	0.0000	C	-3.5441	-2.0002	0.0000	H	-4.8146	1.1611	0.0000
C	0.6327	-1.0334	0.0000	C	-2.1961	-1.7059	0.0000	H	-5.5573	-1.2102	0.0000
C	-0.3385	-0.0434	0.0000	H	5.1051	-2.1430	0.0000	H	-3.8797	-3.0423	0.0000
C	0.0551	1.3252	0.0000	H	5.7854	0.2376	0.0000	H	-1.4414	-2.5074	0.0000

Table 3.42: Table of thermodynamic data as a function of temperature for Benz[*a*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-35.228	287.026	287.026	∞
100	78.069	307.783	607.944	-30.016	310.930	342.301	-178.796
200	149.754	382.483	476.635	-18.830	300.084	377.977	-98.715
250	192.512	420.449	461.583	-10.283	294.927	398.047	-83.166
298.15	234.568	457.958	457.958	0.000	290.300	418.338	-73.290
300	236.169	459.414	457.962	0.435	290.129	419.132	-72.976
350	278.336	499.017	460.994	13.308	285.830	440.981	-65.811
400	317.527	538.780	468.233	28.219	282.063	463.403	-60.513
450	353.078	578.269	478.269	45.000	278.774	486.271	-56.444
500	384.896	617.148	490.220	63.464	275.902	509.497	-53.226
600	438.384	692.242	517.687	104.733	271.193	556.682	-48.462
700	480.881	763.132	547.739	150.775	267.693	604.560	-45.112
800	515.160	829.661	578.866	200.636	265.258	652.854	-42.626
900	543.260	892.013	610.233	253.602	263.750	701.393	-40.707
1000	566.602	950.497	641.366	309.130	263.040	750.066	-39.179
1100	586.189	1005.445	671.992	366.798	262.982	798.782	-37.930
1200	602.756	1057.180	701.957	426.267	263.465	847.467	-36.889
1300	616.859	1105.998	731.177	487.267	264.357	896.102	-36.005
1400	628.936	1152.165	759.614	549.572	265.558	944.660	-35.245
1500	639.330	1195.921	787.255	612.998	267.004	993.123	-34.583
1600	648.322	1237.476	814.106	677.391	268.601	1041.478	-34.000
1700	656.137	1277.020	840.183	742.623	270.293	1089.713	-33.482
1800	662.961	1314.721	865.507	808.586	272.026	1137.891	-33.020
1900	668.946	1350.730	890.105	875.187	273.773	1185.937	-32.603
2000	674.217	1385.179	914.003	942.351	275.495	1233.909	-32.226
2100	678.878	1418.189	937.232	1010.010	277.136	1281.787	-31.882
2200	683.016	1449.868	959.818	1078.109	278.695	1329.591	-31.568
2300	686.703	1480.312	981.791	1146.599	280.165	1377.324	-31.279
2400	690.001	1509.609	1003.177	1215.437	281.497	1424.965	-31.013
2500	692.960	1537.837	1024.002	1284.588	282.698	1472.629	-30.768
2600	695.623	1565.068	1044.292	1354.019	283.741	1520.170	-30.540
2700	698.029	1591.367	1064.070	1423.704	284.630	1567.720	-30.329
2800	700.207	1616.793	1083.358	1493.617	285.345	1615.258	-30.132
2900	702.185	1641.399	1102.179	1563.738	285.866	1662.736	-29.948
3000	703.987	1665.235	1120.552	1634.048	286.222	1710.217	-29.777
3100	705.632	1688.346	1138.498	1704.530	286.360	1757.639	-29.615
3200	707.138	1710.773	1156.032	1775.170	286.308	1805.108	-29.465
3300	708.519	1732.554	1173.174	1845.954	286.052	1852.607	-29.324
3400	709.788	1753.725	1189.940	1916.870	285.574	1900.061	-29.190
3500	710.958	1774.317	1206.343	1987.908	284.876	1947.520	-29.065
3600	712.038	1794.361	1222.400	2059.059	283.973	1995.058	-28.947
3700	713.037	1813.884	1238.123	2130.313	282.843	2042.639	-28.836
3800	713.963	1832.911	1253.526	2201.664	281.468	2090.209	-28.731
3900	714.822	1851.468	1268.621	2273.104	279.876	2137.788	-28.632
4000	715.621	1869.576	1283.420	2344.626	278.054	2185.502	-28.539
4100	716.365	1887.256	1297.933	2416.226	275.980	2233.214	-28.451
4200	717.060	1904.527	1312.170	2487.898	273.672	2280.973	-28.367
4300	717.708	1921.407	1326.143	2559.636	271.118	2328.731	-28.288
4400	718.315	1937.914	1339.860	2631.438	268.328	2376.613	-28.213
4500	718.884	1954.063	1353.330	2703.298	265.308	2424.600	-28.143
4600	719.417	1969.869	1366.562	2775.213	262.025	2472.659	-28.077
4700	719.918	1985.347	1379.564	2847.180	258.488	2520.717	-28.014
4800	720.389	2000.509	1392.343	2919.196	254.730	2568.923	-27.955
4900	720.833	2015.367	1404.906	2991.257	250.699	2617.120	-27.898
5000	721.251	2029.934	1417.262	3063.362	246.460	2665.529	-27.846

3.43. Chrysene



Other names: Benzo[*a*]phenanthrene
1,2-Benzophenanthrene

Formula: C₁₈H₁₂

Mass: 228.288 g/mol

CAS Number: 218-01-9

Point Group: C_{2h}

Length: 13.77 Å

Width: 7.961 Å

Breadth: 3.885 Å

L/B Ratio: 1.729

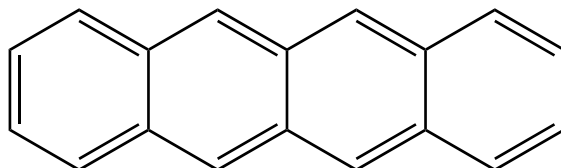
Cartesian coordinates:

C	4.1085	-1.2441	0.0000	C	-1.4781	-2.0631	0.0000	H	4.1673	2.1663	0.0000
C	4.6249	0.0663	0.0000	C	-0.1337	-1.8707	0.0000	H	2.3360	-2.4726	0.0000
C	3.7736	1.1435	0.0000	C	-2.3719	-0.9470	0.0000	H	1.9023	3.0738	0.0000
C	2.7519	-1.4535	0.0000	C	-1.8520	0.3605	0.0000	H	-0.5637	2.7227	0.0000
C	1.8519	-0.3605	0.0000	C	-2.7520	1.4535	0.0000	H	-1.9022	-3.0738	0.0000
C	2.3719	0.9471	0.0000	C	-4.1086	1.2439	0.0000	H	0.5637	-2.7226	0.0000
C	1.4782	2.0632	0.0000	C	-4.6248	-0.0664	0.0000	H	-2.3362	2.4726	0.0000
C	0.1337	1.8708	0.0000	C	-3.7736	-1.1436	0.0000	H	-4.7996	2.0932	0.0000
C	0.4243	-0.5540	0.0000	H	4.7995	-2.0934	0.0000	H	-5.7094	-0.2162	0.0000
C	-0.4243	0.5541	0.0000	H	5.7094	0.2159	0.0000	H	-4.1672	-2.1664	0.0000

Table 3.43: Table of thermodynamic data as a function of temperature for Chrysenes.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-35.475	281.030	281.030	∞
100	79.285	304.944	606.208	-30.126	289.020	320.675	-167.500
200	150.275	380.247	474.535	-18.858	278.256	356.597	-93.132
250	192.777	418.301	459.466	-10.291	273.119	376.776	-78.721
298.15	234.638	455.839	455.839	0.000	268.500	397.170	-69.581
300	236.232	457.295	455.844	0.436	268.330	397.968	-69.291
350	278.262	496.897	458.875	13.308	264.030	419.923	-62.669
400	317.370	536.645	466.113	28.213	260.257	442.451	-57.777
450	352.873	576.112	476.147	44.984	256.958	465.426	-54.024
500	384.665	614.968	488.092	63.438	254.076	488.761	-51.059
600	438.127	690.017	515.547	104.682	249.342	536.165	-46.676
700	480.610	760.866	545.584	150.698	245.816	584.268	-43.598
800	514.877	827.358	576.695	200.531	243.353	632.791	-41.316
900	542.970	889.677	608.046	253.468	241.816	681.562	-39.556
1000	566.310	948.129	639.162	308.967	241.077	730.470	-38.155
1100	585.900	1003.050	669.772	366.605	240.989	779.424	-37.011
1200	602.474	1054.760	699.721	426.047	241.445	828.350	-36.056
1300	616.587	1103.556	728.926	487.018	242.308	877.229	-35.247
1400	628.675	1149.703	757.349	549.297	243.483	926.031	-34.550
1500	639.082	1193.441	784.976	612.697	244.903	974.742	-33.943
1600	648.087	1234.981	811.814	677.066	246.476	1023.345	-33.408
1700	655.916	1274.511	837.879	742.275	248.145	1071.831	-32.933
1800	662.752	1312.200	863.191	808.216	249.856	1120.260	-32.508
1900	668.749	1348.198	887.778	874.798	251.584	1168.559	-32.125
2000	674.032	1382.637	911.666	941.943	253.287	1216.784	-31.778
2100	678.704	1415.639	934.884	1009.584	254.910	1264.917	-31.462
2200	682.853	1447.310	957.461	1077.666	256.452	1312.977	-31.173
2300	686.550	1477.747	979.425	1146.140	257.906	1360.966	-30.908
2400	689.856	1507.037	1000.803	1214.963	259.223	1408.864	-30.662
2500	692.823	1535.260	1021.620	1284.100	260.410	1456.786	-30.437
2600	695.495	1562.486	1041.902	1353.518	261.440	1504.584	-30.227
2700	697.907	1588.780	1061.672	1423.190	262.316	1552.393	-30.032
2800	700.093	1614.201	1080.954	1493.092	263.020	1600.190	-29.851
2900	702.077	1638.804	1099.768	1563.202	263.530	1647.927	-29.682
3000	703.885	1662.636	1118.136	1633.501	263.875	1695.667	-29.524
3100	705.535	1685.744	1136.075	1703.973	264.003	1743.350	-29.375
3200	707.046	1708.168	1153.604	1774.604	263.942	1791.079	-29.236
3300	708.431	1729.946	1170.740	1845.378	263.676	1838.839	-29.106
3400	709.705	1751.114	1187.500	1916.286	263.190	1886.554	-28.983
3500	710.879	1771.704	1203.899	1987.316	262.484	1934.274	-28.867
3600	711.963	1791.745	1219.951	2058.459	261.573	1982.073	-28.759
3700	712.965	1811.266	1235.670	2129.706	260.436	2029.916	-28.657
3800	713.894	1830.292	1251.069	2201.050	259.054	2077.748	-28.560
3900	714.757	1848.847	1266.159	2272.483	257.455	2125.589	-28.468
4000	715.559	1866.954	1280.954	2343.999	255.627	2173.565	-28.383
4100	716.306	1884.632	1295.463	2415.593	253.547	2221.539	-28.302
4200	717.002	1901.901	1309.697	2487.258	251.232	2269.561	-28.226
4300	717.653	1918.781	1323.666	2558.992	248.674	2317.581	-28.152
4400	718.262	1935.286	1337.380	2630.788	245.878	2365.726	-28.084
4500	718.833	1951.434	1350.847	2702.643	242.853	2413.977	-28.020
4600	719.368	1967.239	1364.075	2774.553	239.565	2462.298	-27.960
4700	719.871	1982.715	1377.074	2846.515	236.023	2510.619	-27.902
4800	720.344	1997.876	1389.850	2918.526	232.260	2559.088	-27.848
4900	720.790	2012.734	1402.411	2990.583	228.225	2607.549	-27.796
5000	721.209	2027.300	1414.763	3062.683	223.981	2656.221	-27.749

3.44. Naphthacene



Other names: Benz[*b*]anthracene
2,3-Benzanthracene
Tetracene

Formula: C₁₈H₁₂
Mass: 228.288 g/mol
CAS Number: 92-24-0
Point Group: D_{2h}

Length: 14.05 Å
Width: 7.417 Å
Breadth: 3.882 Å
L/B Ratio: 1.894

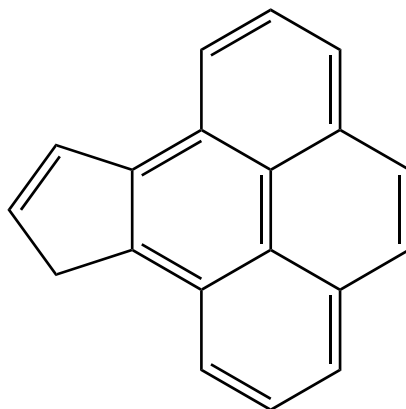
Cartesian coordinates:

C	-4.8585	0.7168	0.0000	C	1.2294	-1.4057	0.0000	H	-3.6825	-2.5010	0.0000
C	-4.8590	-0.7139	0.0000	C	1.2302	1.4050	0.0000	H	-3.6810	2.5032	0.0000
C	-3.6925	-1.4051	0.0000	C	2.4300	0.7144	0.0000	H	-1.2264	-2.5020	0.0000
C	-3.6917	1.4074	0.0000	C	2.4296	-0.7159	0.0000	H	-1.2249	2.5027	0.0000
C	-2.4296	0.7159	0.0000	C	3.6917	-1.4073	0.0000	H	1.2250	-2.5028	0.0000
C	-2.4300	-0.7144	0.0000	C	4.8585	-0.7168	0.0000	H	1.2265	2.5020	0.0000
C	-1.2302	-1.4050	0.0000	C	4.8589	0.7139	0.0000	H	3.6811	-2.5032	0.0000
C	-1.2294	1.4057	0.0000	C	3.6925	1.4051	0.0000	H	5.8211	-1.2385	0.0000
C	0.0002	0.7118	0.0000	H	-5.8211	1.2385	0.0000	H	5.8218	1.2350	0.0000
C	-0.0002	-0.7119	0.0000	H	-5.8219	-1.2349	0.0000	H	3.6825	2.5010	0.0000

Table 3.44: Table of thermodynamic data as a function of temperature for Naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-35.184	320.374	320.374	∞
100	77.427	294.472	595.004	-30.053	340.967	373.669	-195.181
200	150.049	369.054	463.450	-18.879	330.109	410.687	-107.258
250	193.036	407.115	448.358	-10.311	324.973	431.427	-90.140
298.15	235.165	444.724	444.724	0.000	320.374	452.358	-79.250
300	236.766	446.183	444.728	0.437	320.204	453.176	-78.903
350	278.905	485.877	447.767	13.339	315.934	475.685	-70.991
400	318.024	525.712	455.021	28.276	312.194	498.761	-65.130
450	353.495	565.255	465.077	45.080	308.928	522.281	-60.624
500	385.241	604.174	477.047	63.563	306.075	546.157	-57.055
600	438.626	679.320	504.552	104.861	301.395	594.636	-51.767
700	481.067	750.243	534.637	150.924	297.916	643.805	-48.040
800	515.317	816.795	565.792	200.802	295.498	693.387	-45.273
900	543.403	879.165	597.184	253.783	294.005	743.212	-43.134
1000	566.738	937.663	628.338	309.325	293.309	793.168	-41.430
1100	586.320	992.624	658.982	367.006	293.264	843.167	-40.038
1200	602.882	1044.370	688.963	426.489	293.760	893.134	-38.876
1300	616.980	1093.198	718.198	487.500	294.664	943.050	-37.891
1400	629.051	1139.374	746.648	549.817	295.877	992.886	-37.044
1500	639.440	1183.137	774.301	613.254	297.334	1042.628	-36.307
1600	648.426	1224.700	801.163	677.658	298.942	1092.261	-35.658
1700	656.236	1264.250	827.250	742.900	300.644	1141.774	-35.082
1800	663.054	1301.957	852.583	808.873	302.386	1191.229	-34.568
1900	669.034	1337.970	877.189	875.483	304.143	1240.551	-34.104
2000	674.299	1372.423	901.096	942.656	305.873	1289.799	-33.685
2100	678.956	1405.438	924.331	1010.323	307.523	1338.951	-33.304
2200	683.089	1437.120	946.925	1078.429	309.089	1388.031	-32.955
2300	686.772	1467.567	968.904	1146.926	310.566	1437.039	-32.635
2400	690.066	1496.867	990.296	1215.771	311.905	1485.954	-32.340
2500	693.021	1525.098	1011.127	1284.928	313.112	1534.892	-32.069
2600	695.681	1552.331	1031.422	1354.365	314.161	1583.707	-31.816
2700	698.083	1578.632	1051.204	1424.055	315.055	1632.530	-31.583
2800	700.259	1604.060	1070.498	1493.974	315.776	1681.342	-31.365
2900	702.234	1628.668	1089.323	1564.100	316.302	1730.093	-31.162
3000	704.033	1652.505	1107.700	1634.415	316.663	1778.847	-30.972
3100	705.676	1675.618	1125.649	1704.902	316.806	1827.542	-30.793
3200	707.179	1698.046	1143.188	1775.546	316.758	1876.284	-30.627
3300	708.558	1719.829	1160.334	1846.334	316.505	1925.055	-30.470
3400	709.826	1741.000	1177.102	1917.254	316.032	1973.782	-30.323
3500	710.994	1761.593	1193.509	1988.295	315.337	2022.513	-30.184
3600	712.072	1781.638	1209.569	2059.449	314.437	2071.323	-30.054
3700	713.070	1801.162	1225.295	2130.707	313.311	2120.177	-29.931
3800	713.994	1820.191	1240.701	2202.061	311.939	2169.019	-29.815
3900	714.852	1838.748	1255.799	2273.504	310.350	2217.870	-29.704
4000	715.649	1856.857	1270.600	2345.029	308.531	2266.856	-29.601
4100	716.392	1874.537	1285.115	2416.632	306.460	2315.839	-29.504
4200	717.086	1891.809	1299.355	2488.306	304.154	2364.871	-29.411
4300	717.733	1908.690	1313.330	2560.047	301.603	2413.900	-29.322
4400	718.339	1925.198	1327.049	2631.851	298.815	2463.054	-29.240
4500	718.907	1941.347	1340.522	2703.714	295.798	2512.313	-29.162
4600	719.439	1957.154	1353.756	2775.631	292.517	2561.643	-29.088
4700	719.939	1972.632	1366.759	2847.601	288.983	2610.973	-29.017
4800	720.410	1987.794	1379.540	2919.618	285.226	2660.450	-28.951
4900	720.852	2002.653	1392.105	2991.682	281.198	2709.919	-28.887
5000	721.270	2017.220	1404.462	3063.788	276.960	2759.600	-28.829

3.45. 1*H*-Cyclopenta[*e*]pyrene



Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 109587-09-9
Point Group: C_s

Length: 11.01 Å
Width: 10.45 Å
Breadth: 4.177 Å
L/B Ratio: 1.054

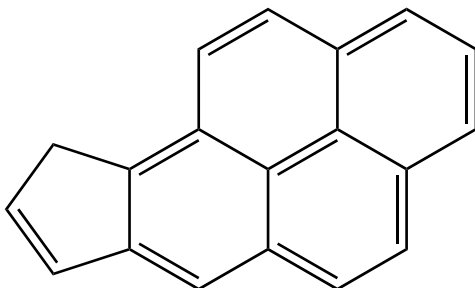
Cartesian coordinates:

C	2.7744	-1.9800	0.0000	C	0.2636	3.5761	0.0000	H	4.9286	-1.2402	0.0000
C	1.5395	-1.1273	-0.0000	C	1.2606	2.6077	-0.0000	H	0.5452	-3.6650	-0.0000
C	1.9027	0.2025	-0.0000	C	-2.1834	-0.8776	0.0000	H	-1.8650	-4.2716	-0.0000
C	3.3625	0.2930	0.0000	C	-2.5453	-2.2286	0.0000	H	-3.6058	-2.5049	0.0000
C	3.8780	-0.9579	0.0000	C	-1.5692	-3.2172	-0.0000	H	-4.2355	-0.1379	0.0000
C	0.1693	-1.5399	-0.0000	C	-0.2211	-2.8815	-0.0000	H	-3.5885	2.2569	0.0000
C	-0.8157	-0.5198	-0.0000	C	-3.1812	0.1620	0.0000	H	-1.8546	3.9853	0.0000
C	-0.4404	0.8667	-0.0000	C	-2.8285	1.4670	0.0000	H	0.5385	4.6362	0.0000
C	0.9245	1.2523	-0.0000	H	2.8243	-2.6352	-0.8892	H	2.3156	2.9048	-0.0000
C	-1.4431	1.8633	0.0000	H	2.8243	-2.6352	0.8892				
C	-1.0769	3.2131	0.0000	H	3.9091	1.2350	0.0000				

Table 3.45: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*e*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-35.668	317.078	317.078	∞
100	76.700	302.593	609.828	-30.723	337.991	369.977	-193.252
200	153.581	378.118	475.062	-19.389	326.968	406.350	-106.126
250	198.245	417.145	459.555	-10.603	321.754	426.800	-89.173
298.15	242.084	455.816	455.816	0.000	317.078	447.466	-78.393
300	243.753	457.319	455.821	0.449	316.905	448.274	-78.050
350	287.726	498.227	458.951	13.747	312.559	470.522	-70.220
400	328.627	539.357	466.432	29.170	308.753	493.347	-64.423
450	365.750	580.246	476.810	46.546	305.431	516.624	-59.967
500	398.983	620.535	489.174	65.680	302.531	540.264	-56.440
600	454.828	698.414	517.613	108.480	297.775	588.280	-51.213
700	499.132	771.981	548.751	156.262	294.241	636.997	-47.532
800	534.782	841.041	581.017	208.019	291.782	686.135	-44.799
900	563.926	905.768	613.543	263.002	290.256	735.519	-42.688
1000	588.066	966.471	645.833	320.638	289.531	785.039	-41.005
1100	608.269	1023.495	677.601	380.484	289.457	834.604	-39.631
1200	625.314	1077.173	708.684	442.187	289.923	884.140	-38.485
1300	639.794	1127.812	738.995	505.462	290.790	933.627	-37.513
1400	652.170	1175.691	768.494	570.076	291.960	983.039	-36.677
1500	662.805	1221.057	797.166	635.838	293.368	1032.359	-35.949
1600	671.992	1264.134	825.016	702.588	294.918	1081.574	-35.309
1700	679.968	1305.118	852.062	770.196	296.553	1130.671	-34.741
1800	686.925	1344.186	878.326	838.548	298.219	1179.717	-34.234
1900	693.020	1381.493	903.834	907.552	299.890	1228.633	-33.777
2000	698.385	1417.179	928.615	977.128	301.525	1277.480	-33.364
2100	703.125	1451.371	952.700	1047.208	303.068	1326.237	-32.988
2200	707.331	1484.179	976.118	1117.735	304.518	1374.926	-32.644
2300	711.077	1515.705	998.897	1188.659	305.869	1423.548	-32.329
2400	714.425	1546.041	1021.067	1259.937	307.071	1472.082	-32.038
2500	717.429	1575.267	1042.654	1331.533	308.131	1520.649	-31.772
2600	720.131	1603.458	1063.684	1403.413	309.024	1569.094	-31.523
2700	722.571	1630.683	1084.183	1475.550	309.751	1617.558	-31.293
2800	724.780	1657.002	1104.173	1547.919	310.294	1666.016	-31.079
2900	726.785	1682.471	1123.678	1620.499	310.632	1714.418	-30.879
3000	728.611	1707.141	1142.718	1693.270	310.795	1762.831	-30.693
3100	730.278	1731.060	1161.313	1766.216	310.729	1811.189	-30.518
3200	731.803	1754.270	1179.482	1839.321	310.462	1859.603	-30.354
3300	733.202	1776.810	1197.243	1912.573	309.981	1908.056	-30.201
3400	734.488	1798.718	1214.612	1985.958	309.268	1956.467	-30.057
3500	735.672	1820.026	1231.607	2059.467	308.323	2004.889	-29.921
3600	736.765	1840.766	1248.241	2133.089	307.164	2053.402	-29.793
3700	737.776	1860.967	1264.530	2206.817	305.768	2101.964	-29.674
3800	738.713	1880.654	1280.485	2280.642	304.115	2150.522	-29.560
3900	739.583	1899.854	1296.122	2354.557	302.235	2199.093	-29.453
4000	740.391	1918.589	1311.450	2428.557	300.116	2247.812	-29.353
4100	741.144	1936.881	1326.482	2502.634	297.734	2296.534	-29.258
4200	741.847	1954.749	1341.229	2576.784	295.107	2345.311	-29.168
4300	742.503	1972.213	1355.701	2651.002	292.224	2394.091	-29.082
4400	743.117	1989.290	1369.907	2725.283	289.095	2443.006	-29.002
4500	743.692	2005.996	1383.858	2799.624	285.726	2492.035	-28.926
4600	744.231	2022.348	1397.561	2874.020	282.084	2541.145	-28.855
4700	744.738	2038.359	1411.025	2948.469	278.176	2590.258	-28.787
4800	745.214	2054.043	1424.258	3022.967	274.038	2639.531	-28.723
4900	745.663	2069.413	1437.268	3097.511	269.616	2688.798	-28.662
5000	746.086	2084.482	1450.063	3172.098	264.977	2738.291	-28.606

3.46. 1*H*-Cyclopenta[*a*]pyrene



Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 42315-22-0
Point Group: C_s

Length: 13.08 Å
Width: 9.203 Å
Breadth: 4.175 Å
L/B Ratio: 1.421

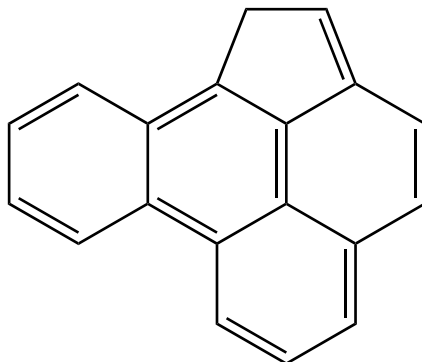
Cartesian coordinates:

C	-2.3912	-1.0205	0.0000	C	-0.9799	2.4620	0.0000	H	3.4251	2.1362	0.8884
C	-1.8942	-2.3723	0.0000	C	0.3491	2.2153	0.0000	H	2.1383	-2.8674	0.0000
C	-0.5658	-2.6264	0.0000	C	-3.7625	-0.7452	0.0000	H	-2.6256	-3.1886	0.0000
C	0.4005	-1.5574	0.0000	C	-4.2124	0.5688	0.0000	H	-0.1899	-3.6561	0.0000
C	-0.0592	-0.2189	0.0000	C	-3.3118	1.6281	0.0000	H	1.0800	3.0322	0.0000
C	-1.4674	0.0489	0.0000	C	4.1259	-0.7651	0.0000	H	-1.3641	3.4884	0.0000
C	0.8550	0.8667	0.0000	C	4.5624	0.5123	0.0000	H	-3.6792	2.6606	0.0000
C	2.2126	0.5695	0.0000	C	3.4069	1.4780	-0.0000	H	-5.2883	0.7733	0.0000
C	2.6613	-0.7712	0.0000	H	4.7252	-1.6740	0.0000	H	-4.4813	-1.5723	0.0000
C	1.7755	-1.8340	0.0000	H	5.5953	0.8551	0.0000				
C	-1.9363	1.3831	0.0000	H	3.4251	2.1362	-0.8884				

Table 3.46: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*a*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-35.894	314.643	314.643	∞
100	77.177	304.168	613.065	-30.890	335.390	367.218	-191.811
200	154.429	380.076	477.564	-19.498	324.424	403.415	-105.359
250	199.378	419.325	461.970	-10.661	319.261	423.761	-88.538
298.15	243.370	458.211	458.211	0.000	314.643	444.317	-77.841
300	245.043	459.721	458.215	0.452	314.473	445.121	-77.501
350	289.063	500.833	461.362	13.815	310.193	467.243	-69.731
400	329.941	542.141	468.878	29.305	306.453	489.934	-63.977
450	367.004	583.181	479.303	46.745	303.195	513.068	-59.554
500	400.159	623.598	491.718	65.940	300.356	536.557	-56.053
600	455.844	701.678	520.261	108.850	295.710	584.257	-50.863
700	500.009	775.391	551.497	156.726	292.270	632.640	-47.207
800	535.548	844.560	583.854	208.565	289.893	681.430	-44.492
900	564.601	909.372	616.461	263.620	288.439	730.459	-42.394
1000	588.667	970.142	648.823	321.320	287.778	779.614	-40.722
1100	608.807	1027.221	680.655	381.223	287.760	828.810	-39.356
1200	625.799	1080.943	711.796	442.976	288.277	877.971	-38.216
1300	640.233	1131.619	742.159	506.297	289.191	927.079	-37.250
1400	652.569	1179.528	771.705	570.953	290.403	976.109	-36.418
1500	663.168	1224.922	800.419	636.753	291.849	1025.044	-35.694
1600	672.324	1268.021	828.309	703.539	293.434	1073.871	-35.058
1700	680.272	1309.024	855.390	771.178	295.101	1122.579	-34.492
1800	687.204	1348.108	881.686	839.559	296.795	1171.233	-33.988
1900	693.278	1385.430	907.224	908.590	298.493	1219.756	-33.533
2000	698.622	1421.129	932.034	978.191	300.153	1268.209	-33.122
2100	703.345	1455.331	956.144	1048.294	301.719	1316.570	-32.747
2200	707.535	1488.150	979.585	1118.842	303.190	1364.862	-32.405
2300	711.267	1519.685	1002.387	1189.786	304.561	1413.087	-32.092
2400	714.602	1550.028	1024.577	1261.082	305.781	1461.223	-31.802
2500	717.593	1579.261	1046.183	1332.695	306.858	1509.391	-31.536
2600	720.285	1607.459	1067.232	1404.591	307.767	1557.436	-31.289
2700	722.715	1634.689	1087.747	1476.743	308.509	1605.500	-31.060
2800	724.915	1661.013	1107.754	1549.126	309.066	1653.556	-30.847
2900	726.913	1686.487	1127.273	1621.719	309.417	1701.558	-30.648
3000	728.731	1711.161	1146.327	1694.503	309.593	1749.568	-30.462
3100	730.391	1735.084	1164.935	1767.460	309.538	1797.524	-30.287
3200	731.910	1758.297	1183.117	1840.576	309.282	1845.536	-30.125
3300	733.303	1780.841	1200.890	1913.838	308.812	1893.586	-29.972
3400	734.583	1802.751	1218.271	1987.233	308.108	1941.593	-29.828
3500	735.763	1824.062	1235.276	2060.751	307.173	1989.612	-29.693
3600	736.851	1844.805	1251.921	2134.383	306.023	2037.721	-29.566
3700	737.858	1865.008	1268.219	2208.119	304.635	2085.879	-29.447
3800	738.791	1884.697	1284.184	2281.952	302.990	2134.033	-29.334
3900	739.657	1903.899	1299.829	2355.875	301.118	2182.200	-29.227
4000	740.462	1922.636	1315.166	2429.881	299.006	2230.514	-29.127
4100	741.212	1940.929	1330.206	2503.965	296.630	2278.831	-29.032
4200	741.911	1958.799	1344.961	2578.122	294.010	2327.204	-28.942
4300	742.565	1976.264	1359.440	2652.346	291.134	2375.579	-28.857
4400	743.176	1993.343	1373.653	2726.633	288.010	2424.088	-28.777
4500	743.748	2010.050	1387.610	2800.980	284.648	2472.712	-28.702
4600	744.285	2026.403	1401.320	2875.382	281.011	2521.417	-28.631
4700	744.790	2042.415	1414.791	2949.836	277.109	2570.124	-28.563
4800	745.264	2058.101	1428.030	3024.339	272.976	2618.991	-28.500
4900	745.711	2073.472	1441.046	3098.888	268.559	2667.852	-28.439
5000	746.132	2088.542	1453.846	3173.480	263.924	2716.939	-28.383

3.47. 1*H*-Benz[*fg*]aceanthrylene



Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 193-69-1
Point Group: C_s

Length: 11.88 Å
Width: 10.40 Å
Breadth: 4.178 Å
L/B Ratio: 1.143

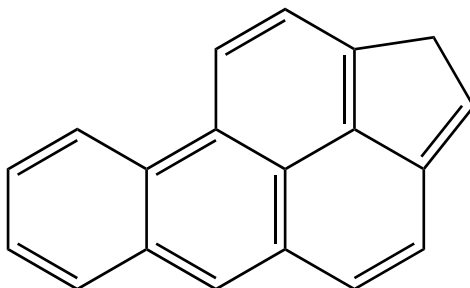
Cartesian coordinates:

C	-2.4672	-2.3605	-0.0000	C	1.6355	0.7070	-0.0000	H	-4.4011	-0.4309	-0.0000
C	-2.2920	-0.9837	-0.0000	C	0.4577	1.5197	0.0000	H	-4.0384	2.0187	-0.0000
C	-0.9662	-0.4942	0.0000	C	2.9289	1.2657	-0.0000	H	3.0333	2.3565	-0.0000
C	0.1663	-1.3219	0.0000	C	4.0398	0.4514	-0.0000	H	5.0439	0.8878	-0.0000
C	-0.0565	-2.7113	0.0000	C	3.8930	-0.9444	-0.0000	H	4.7839	-1.5807	-0.0000
C	-1.3482	-3.2073	0.0000	C	2.6371	-1.5100	0.0000	H	2.5031	-2.6031	0.0000
C	-0.7674	0.9037	0.0000	C	-1.3037	3.1104	0.0000	H	0.8169	-3.3806	0.0000
C	-1.8555	1.8669	0.0000	C	0.2091	3.0035	0.0000	H	-1.5071	-4.2911	0.0000
C	-3.1944	1.3216	-0.0000	H	0.6454	3.4938	-0.8895	H	-3.4749	-2.7899	-0.0000
C	-3.3855	-0.0178	-0.0000	H	0.6454	3.4938	0.8895				
C	1.4814	-0.7032	0.0000	H	-1.8166	4.0692	-0.0000				

Table 3.47: Table of thermodynamic data as a function of temperature for 1*H*-Benz[*fg*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-36.044	362.825	362.825	∞
100	77.988	304.821	614.679	-30.986	383.477	415.239	-216.894
200	154.902	381.187	478.835	-19.530	372.575	451.343	-117.876
250	199.695	420.525	463.219	-10.674	367.431	471.631	-98.540
298.15	243.570	459.456	459.456	0.000	362.825	492.128	-86.217
300	245.239	460.967	459.460	0.452	362.656	492.930	-85.825
350	289.172	502.103	462.609	13.823	358.383	514.989	-76.856
400	329.987	543.421	470.128	29.317	354.647	537.616	-70.204
450	367.003	584.463	480.556	46.758	351.390	560.686	-65.081
500	400.125	624.879	492.974	65.952	348.551	584.111	-61.020
600	455.766	702.948	521.521	108.856	343.898	631.683	-54.992
700	499.905	776.646	552.757	156.722	340.450	679.940	-50.737
800	535.428	845.801	585.112	208.551	338.061	728.606	-47.572
900	564.474	910.597	617.717	263.593	336.594	777.511	-45.125
1000	588.537	971.355	650.075	321.280	335.920	826.545	-43.173
1100	608.678	1028.421	681.903	381.170	335.890	875.620	-41.579
1200	625.673	1082.132	713.039	442.911	336.394	924.661	-40.249
1300	640.112	1132.798	743.398	506.219	337.296	973.651	-39.121
1400	652.452	1180.698	772.939	570.863	338.496	1022.563	-38.152
1500	663.058	1226.084	801.649	636.652	339.930	1071.382	-37.308
1600	672.220	1269.176	829.534	703.427	341.504	1120.093	-36.567
1700	680.174	1310.173	856.611	771.056	343.161	1168.686	-35.909
1800	687.112	1349.252	882.903	839.428	344.846	1217.226	-35.322
1900	693.192	1386.569	908.437	908.450	346.535	1265.634	-34.794
2000	698.542	1422.264	933.243	978.042	348.186	1313.973	-34.317
2100	703.269	1456.462	957.349	1048.137	349.745	1362.221	-33.883
2200	707.464	1489.277	980.787	1118.678	351.208	1410.401	-33.486
2300	711.200	1520.809	1003.585	1189.615	352.572	1458.513	-33.123
2400	714.539	1551.149	1025.772	1260.905	353.786	1506.537	-32.788
2500	717.535	1580.380	1047.376	1332.511	354.858	1554.592	-32.481
2600	720.230	1608.576	1068.421	1404.402	355.760	1602.526	-32.194
2700	722.663	1635.804	1088.934	1476.548	356.497	1650.478	-31.930
2800	724.866	1662.126	1108.938	1548.927	357.049	1698.423	-31.684
2900	726.866	1687.598	1128.455	1621.515	357.395	1746.313	-31.454
3000	728.687	1712.271	1147.506	1694.294	357.566	1794.213	-31.239
3100	730.349	1736.192	1166.112	1767.247	357.507	1842.057	-31.038
3200	731.870	1759.404	1184.292	1840.359	357.248	1889.958	-30.850
3300	733.265	1781.946	1202.063	1913.617	356.773	1937.898	-30.674
3400	734.548	1803.856	1219.442	1987.008	356.066	1985.795	-30.507
3500	735.729	1825.166	1236.445	2060.523	355.127	2033.703	-30.351
3600	736.819	1845.907	1253.088	2134.151	353.974	2081.702	-30.204
3700	737.827	1866.109	1269.384	2207.884	352.583	2129.750	-30.066
3800	738.762	1885.799	1285.348	2281.714	350.935	2177.794	-29.935
3900	739.629	1905.000	1300.991	2355.634	349.060	2225.850	-29.811
4000	740.435	1923.736	1316.326	2429.638	346.945	2274.054	-29.695
4100	741.186	1942.028	1331.365	2503.719	344.567	2322.262	-29.585
4200	741.887	1959.898	1346.118	2577.874	341.944	2370.524	-29.481
4300	742.541	1977.362	1360.596	2652.095	339.066	2418.789	-29.382
4400	743.153	1994.440	1374.808	2726.380	335.940	2467.189	-29.289
4500	743.727	2011.147	1388.764	2800.725	332.575	2515.703	-29.201
4600	744.265	2027.500	1402.473	2875.124	328.936	2564.298	-29.118
4700	744.770	2043.511	1415.942	2949.576	325.032	2612.896	-29.038
4800	745.245	2059.196	1429.180	3024.077	320.897	2661.653	-28.964
4900	745.693	2074.567	1442.195	3098.625	316.478	2710.405	-28.893
5000	746.114	2089.637	1454.994	3173.215	311.842	2759.383	-28.826

3.48. 1*H*-Indeno[6,7,1-*mna*]anthracene



Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 190-12-5
Point Group: C_s

Length: 12.84 Å
Width: 9.203 Å
Breadth: 4.177 Å
L/B Ratio: 1.395

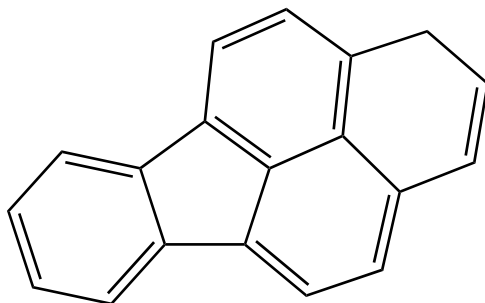
Cartesian coordinates:

C	-4.0911	0.1184	-0.0000	C	4.5348	0.2576	0.0000	H	-0.9390	3.6103	0.0000
C	-3.8133	-1.3744	0.0000	C	3.5617	1.2307	0.0000	H	-3.3271	2.9646	-0.0000
C	-2.9242	0.8133	-0.0000	C	0.4467	-0.8570	-0.0000	H	1.5129	2.9567	0.0000
C	-1.2295	2.5529	0.0000	C	-0.4869	0.1886	0.0000	H	2.5462	-2.5256	-0.0000
C	-2.5365	2.2074	-0.0000	C	-1.8357	-0.1505	-0.0000	H	4.9655	-1.8650	-0.0000
C	-0.1361	1.5825	0.0000	C	-2.3104	-1.4576	0.0000	H	5.5936	0.5366	0.0000
C	1.1885	1.9092	0.0000	C	-1.3782	-2.5016	0.0000	H	3.8398	2.2909	0.0000
C	2.1928	0.8791	-0.0000	C	-0.0256	-2.1914	0.0000	H	-1.7108	-3.5439	0.0000
C	1.8416	-0.4875	-0.0000	H	-5.1037	0.5155	-0.0000	H	0.7326	-2.9899	-0.0000
C	2.8543	-1.4686	-0.0000	H	-4.2524	-1.8620	-0.8893				
C	4.1803	-1.1022	0.0000	H	-4.2524	-1.8620	0.8893				

Table 3.48: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[6,7,1-*mna*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-35.804	358.491	358.491	∞
100	76.926	304.388	612.314	-30.793	379.335	411.141	-214.754
200	153.879	379.948	477.210	-19.453	368.317	447.334	-116.829
250	198.927	419.085	461.649	-10.641	363.129	467.689	-97.716
298.15	242.972	457.897	457.897	0.000	358.491	488.258	-85.539
300	244.645	459.405	457.902	0.451	358.320	489.063	-85.152
350	288.676	500.457	461.043	13.795	354.021	511.202	-76.291
400	329.544	541.713	468.549	29.265	350.261	533.913	-69.720
450	366.593	582.705	478.960	46.685	346.983	557.070	-64.662
500	399.741	623.079	491.359	65.860	344.123	580.584	-60.652
600	455.431	701.082	519.869	108.728	339.435	628.340	-54.701
700	499.622	774.733	551.072	156.563	335.956	676.786	-50.501
800	535.195	843.853	583.396	208.366	333.541	725.645	-47.379
900	564.284	908.624	615.973	263.386	332.053	774.746	-44.964
1000	588.384	969.364	648.307	321.057	331.362	823.978	-43.039
1100	608.555	1026.416	680.114	380.933	331.318	873.253	-41.466
1200	625.575	1080.118	711.232	442.663	331.811	922.495	-40.154
1300	640.033	1130.777	741.575	505.962	332.704	971.687	-39.042
1400	652.389	1178.672	771.101	570.599	333.897	1020.801	-38.086
1500	663.006	1224.054	799.799	636.382	335.326	1069.822	-37.254
1600	672.178	1267.143	827.673	703.152	336.895	1118.737	-36.522
1700	680.140	1308.138	854.739	770.778	338.548	1167.533	-35.873
1800	687.084	1347.215	881.022	839.146	340.230	1216.276	-35.295
1900	693.168	1384.530	906.548	908.166	341.916	1264.889	-34.774
2000	698.522	1420.224	931.346	977.756	343.565	1313.432	-34.303
2100	703.253	1454.422	955.446	1047.849	345.122	1361.884	-33.874
2200	707.450	1487.236	978.877	1118.388	346.584	1410.267	-33.483
2300	711.188	1518.767	1001.670	1189.324	347.947	1458.584	-33.125
2400	714.529	1549.107	1023.852	1260.613	349.160	1506.812	-32.794
2500	717.526	1578.337	1045.450	1332.218	350.230	1555.072	-32.491
2600	720.222	1606.533	1066.491	1404.108	351.132	1603.209	-32.208
2700	722.656	1633.761	1087.000	1476.254	351.868	1651.365	-31.947
2800	724.860	1660.082	1107.000	1548.632	352.419	1699.515	-31.704
2900	726.861	1685.554	1126.513	1621.219	352.765	1747.610	-31.477
3000	728.683	1710.227	1145.561	1693.998	352.936	1795.714	-31.266
3100	730.346	1734.148	1164.164	1766.951	352.876	1843.763	-31.067
3200	731.867	1757.360	1182.340	1840.062	352.616	1891.868	-30.881
3300	733.262	1779.902	1200.108	1913.320	352.142	1940.012	-30.707
3400	734.545	1801.812	1217.485	1986.711	351.434	1988.114	-30.543
3500	735.727	1823.122	1234.486	2060.225	350.495	2036.226	-30.388
3600	736.817	1843.863	1251.126	2133.853	349.341	2084.429	-30.244
3700	737.826	1864.065	1267.420	2207.586	347.950	2132.682	-30.107
3800	738.760	1883.754	1283.381	2281.416	346.302	2180.930	-29.978
3900	739.628	1902.955	1299.023	2355.336	344.427	2229.191	-29.856
4000	740.434	1921.691	1314.356	2429.340	342.312	2277.600	-29.742
4100	741.185	1939.984	1329.393	2503.421	339.934	2326.011	-29.633
4200	741.886	1957.853	1344.145	2577.575	337.311	2374.478	-29.530
4300	742.540	1975.318	1358.621	2651.797	334.432	2422.948	-29.432
4400	743.153	1992.395	1372.831	2726.082	331.306	2471.552	-29.340
4500	743.726	2009.103	1386.786	2800.426	327.942	2520.271	-29.254
4600	744.264	2025.455	1400.493	2874.826	324.302	2569.070	-29.172
4700	744.769	2041.467	1413.961	2949.278	320.398	2617.872	-29.094
4800	745.245	2057.152	1427.198	3023.778	316.263	2666.834	-29.020
4900	745.692	2072.523	1440.211	3098.326	311.844	2715.790	-28.950
5000	746.114	2087.592	1453.009	3172.916	307.208	2764.973	-28.885

3.49. 1*H*-Benzo[*cd*]fluoranthene



Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 42126-84-1
Point Group: C_s

Length: 13.20 Å
Width: 9.179 Å
Breadth: 4.170 Å
L/B Ratio: 1.438

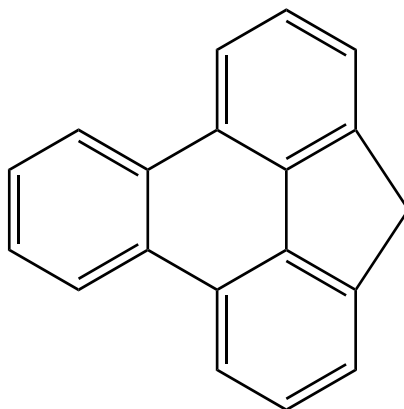
Cartesian coordinates:

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C	2.0904	-0.5592	0.0000	C	0.1843	-2.3846	0.0000	H	0.3125	3.3738	0.0000
C	3.3285	-1.1679	0.0000	C	-2.0790	-1.4205	0.0000	H	-2.1670	3.2449	0.0000
C	4.4695	-0.3559	0.0000	C	-1.5212	-0.1122	0.0000	H	-1.6614	-3.5205	0.0000
C	4.3650	1.0274	-0.0000	C	-2.2651	1.1032	0.0000	H	0.8078	-3.2842	0.0000
C	3.1151	1.6589	0.0000	C	-3.7122	0.9672	0.0000	H	-4.3079	1.8870	0.0000
C	0.5588	1.2346	0.0000	C	-4.2941	-0.2412	-0.0000	H	-5.3876	-0.3225	-0.0000
C	-0.1732	2.3929	0.0000	C	-3.5651	-1.5409	-0.0000	H	-3.8863	-2.1277	0.8858
C	-1.5934	2.3110	0.0000	H	3.4165	-2.2589	0.0000	H	-3.8863	-2.1277	-0.8858
C	0.7371	-1.1318	0.0000	H	5.4589	-0.8250	-0.0000				
C	-0.1430	-0.0084	0.0000	H	5.2728	1.6397	-0.0000				

Table 3.49: Table of thermodynamic data as a function of temperature for 1*H*-Benzo[*cd*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-36.068	351.144	351.144	∞
100	79.580	307.400	616.101	-30.870	371.911	403.416	-210.718
200	154.105	384.013	480.973	-19.392	361.031	439.234	-114.714
250	198.250	423.099	465.470	-10.593	355.830	459.387	-95.982
298.15	241.693	461.736	461.736	0.000	351.144	479.767	-84.051
300	243.349	463.236	461.741	0.449	350.971	480.564	-83.672
350	287.017	504.058	464.865	13.718	346.597	502.518	-74.995
400	327.716	545.079	472.328	29.100	342.749	525.055	-68.564
450	364.727	585.853	482.681	46.427	339.378	548.049	-63.615
500	397.918	626.032	495.013	65.509	336.426	571.410	-59.694
600	453.822	703.720	523.379	108.205	331.566	618.887	-53.878
700	498.278	777.143	554.439	155.892	327.938	667.081	-49.777
800	534.104	846.100	586.633	207.574	325.402	715.708	-46.730
900	563.411	910.756	619.093	262.497	323.817	764.590	-44.375
1000	587.688	971.413	651.325	320.089	323.047	813.613	-42.498
1100	608.000	1028.406	683.041	379.902	322.941	862.687	-40.965
1200	625.130	1082.064	714.079	441.583	323.385	911.732	-39.686
1300	639.675	1132.691	744.351	504.842	324.237	960.731	-38.602
1400	652.100	1180.563	773.815	569.447	325.398	1009.655	-37.670
1500	662.771	1225.926	802.457	635.204	326.801	1058.488	-36.859
1600	671.985	1269.002	830.281	701.953	328.349	1107.216	-36.146
1700	679.980	1309.986	857.304	769.560	329.984	1155.827	-35.514
1800	686.951	1349.055	883.546	837.915	331.652	1204.386	-34.950
1900	693.057	1386.363	909.036	906.922	333.326	1252.815	-34.442
2000	698.428	1422.052	933.801	976.502	334.964	1301.175	-33.982
2100	703.173	1456.246	957.871	1046.587	336.512	1349.444	-33.565
2200	707.382	1489.056	981.275	1117.118	337.967	1397.645	-33.184
2300	711.130	1520.585	1004.042	1188.048	339.323	1445.780	-32.834
2400	714.479	1550.922	1026.201	1259.331	340.531	1493.826	-32.512
2500	717.482	1580.151	1047.778	1330.932	341.597	1541.905	-32.216
2600	720.185	1608.345	1068.799	1402.818	342.494	1589.861	-31.940
2700	722.623	1635.571	1089.290	1474.960	343.227	1637.836	-31.685
2800	724.831	1661.892	1109.272	1547.335	343.775	1685.805	-31.448
2900	726.836	1687.363	1128.770	1619.920	344.118	1733.719	-31.227
3000	728.660	1712.035	1147.803	1692.696	344.287	1781.642	-31.020
3100	730.325	1735.955	1166.391	1765.646	344.225	1829.510	-30.826
3200	731.849	1759.166	1184.555	1838.756	343.963	1877.435	-30.645
3300	733.246	1781.708	1202.310	1912.012	343.487	1925.398	-30.476
3400	734.531	1803.617	1219.675	1985.402	342.777	1973.319	-30.316
3500	735.714	1824.926	1236.665	2058.915	341.837	2021.251	-30.165
3600	736.805	1845.668	1253.295	2132.541	340.682	2069.274	-30.024
3700	737.815	1865.869	1269.579	2206.273	339.290	2117.346	-29.891
3800	738.751	1885.558	1285.531	2280.102	337.641	2165.414	-29.765
3900	739.619	1904.759	1301.164	2354.021	335.765	2213.494	-29.646
4000	740.426	1923.495	1316.489	2428.024	333.649	2261.723	-29.534
4100	741.178	1941.787	1331.518	2502.104	331.270	2309.954	-29.429
4200	741.879	1959.656	1346.262	2576.257	328.646	2358.241	-29.328
4300	742.534	1977.121	1360.730	2650.478	325.767	2406.530	-29.233
4400	743.147	1994.198	1374.934	2724.763	322.641	2454.954	-29.143
4500	743.721	2010.905	1388.882	2799.107	319.275	2503.492	-29.059
4600	744.259	2027.258	1402.582	2873.506	315.636	2552.112	-28.980
4700	744.765	2043.269	1416.044	2947.957	311.731	2600.733	-28.903
4800	745.240	2058.954	1429.275	3022.458	307.596	2649.515	-28.832
4900	745.688	2074.325	1442.283	3097.004	303.176	2698.291	-28.764
5000	746.110	2089.394	1455.075	3171.595	298.539	2747.293	-28.700

3.50. 4*H*-Cyclopenta[*def*]triphenylene



Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 23992-32-7
Point Group: C_{2v}

Length: 11.69 Å
Width: 10.46 Å
Breadth: 4.178 Å
L/B Ratio: 1.117

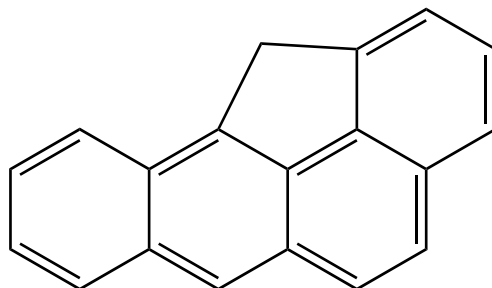
Cartesian coordinates:

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C	0.6841	2.7782	0.0000	C	1.6144	0.3575	0.0000	H	-3.9902	-2.1818	-0.0000
C	-0.4591	3.5665	0.0000	C	1.2947	-1.0282	0.0000	H	-2.3489	-4.0350	0.0000
C	-1.7679	3.0380	-0.0000	C	2.3368	-1.9674	-0.0000	H	0.0934	-3.6457	0.0000
C	0.5663	1.3745	0.0000	C	3.6586	-1.5606	-0.0000	H	2.0848	-3.0363	-0.0000
C	-0.7334	0.9006	0.0000	C	3.9726	-0.1999	-0.0000	H	4.4617	-2.3048	-0.0000
C	-0.0928	-1.4834	0.0000	C	2.9626	0.7450	-0.0000	H	5.0205	0.1172	-0.0000
C	-1.0537	-0.4882	0.0000	H	-3.7366	0.8616	-0.8896	H	3.2050	1.8161	-0.0000
C	-2.4527	-0.6604	-0.0000	H	-3.7366	0.8616	0.8896				
C	-2.9197	-1.9570	-0.0000	H	1.6802	3.2373	0.0000				

Table 3.50: Table of thermodynamic data as a function of temperature for 4*H*-Cyclopenta[*def*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-35.637	307.386	307.386	∞
100	77.441	299.342	605.129	-30.579	328.445	360.755	-188.435
200	152.669	374.775	471.109	-19.267	317.398	397.449	-103.801
250	196.968	413.556	455.700	-10.536	312.129	418.072	-87.350
298.15	240.621	451.985	451.985	0.000	307.386	438.917	-76.895
300	242.285	453.478	451.989	0.447	307.211	439.732	-76.563
350	286.196	494.154	455.101	13.669	302.790	462.178	-68.975
400	327.115	535.081	462.541	29.016	298.907	485.212	-63.361
450	364.303	575.794	472.867	46.318	295.511	508.708	-59.048
500	397.623	615.936	485.172	65.382	292.541	532.573	-55.636
600	453.662	693.584	513.492	108.056	287.659	581.062	-50.585
700	498.148	766.985	544.515	155.729	284.018	630.271	-47.030
800	533.954	835.924	576.679	207.397	281.468	679.914	-44.393
900	563.227	900.561	609.113	262.303	279.865	729.815	-42.356
1000	587.473	961.197	641.322	319.875	279.076	779.859	-40.735
1100	607.761	1018.168	673.017	379.666	278.947	829.955	-39.410
1200	624.877	1071.805	704.037	441.322	279.366	880.025	-38.306
1300	639.415	1122.411	734.292	504.555	280.193	930.051	-37.369
1400	651.838	1170.263	763.739	569.134	281.327	980.004	-36.564
1500	662.513	1215.609	792.365	634.865	282.704	1029.868	-35.862
1600	671.733	1258.668	820.175	701.588	284.226	1079.628	-35.246
1700	679.737	1299.637	847.184	769.171	285.837	1129.273	-34.698
1800	686.718	1338.692	873.413	837.501	287.481	1178.868	-34.209
1900	692.834	1375.988	898.890	906.486	289.132	1228.334	-33.769
2000	698.216	1411.666	923.644	976.044	290.749	1277.732	-33.370
2100	702.972	1445.849	947.702	1046.108	292.276	1327.040	-33.008
2200	707.191	1478.651	971.096	1116.620	293.712	1376.282	-32.676
2300	710.949	1510.171	993.853	1187.531	295.049	1425.458	-32.372
2400	714.307	1540.501	1016.002	1258.797	296.239	1474.545	-32.092
2500	717.320	1569.723	1037.570	1330.381	297.288	1523.666	-31.835
2600	720.030	1597.910	1058.583	1402.251	298.170	1572.666	-31.595
2700	722.477	1625.131	1079.065	1474.378	298.887	1621.685	-31.373
2800	724.693	1651.447	1099.040	1546.738	299.422	1670.698	-31.167
2900	726.704	1676.913	1118.530	1619.310	299.751	1719.656	-30.974
3000	728.535	1701.580	1137.556	1692.073	299.906	1768.624	-30.794
3100	730.207	1725.497	1156.138	1765.012	299.833	1817.538	-30.625
3200	731.736	1748.704	1174.295	1838.110	299.559	1866.509	-30.467
3300	733.139	1771.243	1192.044	1911.355	299.072	1915.518	-30.320
3400	734.428	1793.148	1209.403	1984.734	298.352	1964.486	-30.180
3500	735.616	1814.455	1226.387	2058.237	297.402	2013.466	-30.049
3600	736.712	1835.194	1243.012	2131.854	296.237	2062.535	-29.926
3700	737.726	1855.393	1259.291	2205.577	294.836	2111.655	-29.811
3800	738.666	1875.079	1275.238	2279.397	293.178	2160.770	-29.701
3900	739.538	1894.278	1290.866	2353.308	291.294	2209.899	-29.598
4000	740.349	1913.012	1306.186	2427.302	289.171	2259.176	-29.501
4100	741.104	1931.302	1321.211	2501.375	286.784	2308.456	-29.409
4200	741.808	1949.170	1335.950	2575.521	284.153	2357.791	-29.323
4300	742.466	1966.633	1350.415	2649.735	281.267	2407.129	-29.240
4400	743.081	1983.709	1364.615	2724.013	278.133	2456.602	-29.163
4500	743.658	2000.414	1378.559	2798.350	274.762	2506.189	-29.090
4600	744.199	2016.765	1392.256	2872.744	271.116	2555.857	-29.022
4700	744.707	2032.775	1405.714	2947.189	267.205	2605.529	-28.957
4800	745.184	2048.459	1418.942	3021.684	263.064	2655.360	-28.896
4900	745.634	2063.829	1431.946	3096.225	258.639	2705.185	-28.837
5000	746.058	2078.897	1444.735	3170.810	253.997	2755.237	-28.783

3.51. 1*H*-Benz[*bc*]aceanthrylene



Other names: 1',9-Methylene-1,2-benzanthracene

Formula: C₁₉H₁₂

Mass: 240.299 g/mol

CAS Number: 202-94-8

Point Group: C_s

Length: 13.37 Å

Width: 8.964 Å

Breadth: 4.178 Å

L/B Ratio: 1.492

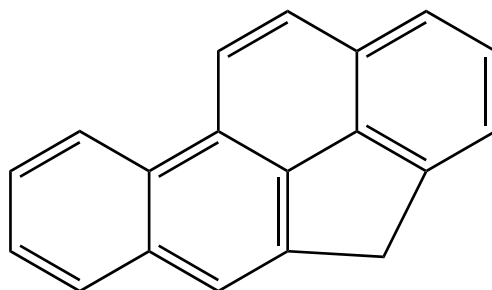
Cartesian coordinates:

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C	-4.0318	-0.2168	-0.0029	C	2.3126	-0.7853	-0.0017	H	-0.8037	-3.6559	-0.0051
C	-4.1577	1.1656	0.0019	C	1.8791	0.5768	0.0026	H	-3.1678	-2.9395	-0.0112
C	-3.0568	2.0526	0.0050	C	2.8461	1.6241	0.0057	H	1.8002	-2.9014	-0.0072
C	-2.7478	-0.7981	-0.0037	C	4.1783	1.3351	0.0033	H	2.4883	2.6598	0.0097
C	-1.7007	0.1077	-0.0001	C	4.6191	-0.0148	-0.0012	H	4.9250	2.1357	0.0046
C	-1.0593	-2.5905	-0.0055	C	3.7196	-1.0395	-0.0035	H	5.6951	-0.2178	-0.0023
C	-2.3634	-2.1958	-0.0070	H	-0.1805	2.6960	-0.8828	H	4.0623	-2.0809	-0.0061
C	0.0406	-1.6440	-0.0026	H	-0.1807	2.6933	0.8960				
C	-0.3346	-0.2941	0.0006	H	-4.9204	-0.8561	-0.0050				

Table 3.51: Table of thermodynamic data as a function of temperature for 1*H*-Benz[*bc*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-35.794	330.106	330.106	∞
100	77.420	305.653	612.978	-30.733	351.011	382.691	-199.893
200	153.504	381.273	478.217	-19.389	339.997	418.748	-109.364
250	198.253	420.293	462.709	-10.604	334.781	439.040	-91.730
298.15	242.127	458.969	458.969	0.000	330.106	459.554	-80.510
300	243.796	460.472	458.974	0.449	329.934	460.357	-80.154
350	287.757	501.387	462.105	13.749	325.590	482.447	-72.000
400	328.628	542.519	469.586	29.173	321.785	505.114	-65.960
450	365.721	583.406	479.966	46.548	318.462	528.233	-61.314
500	398.932	623.691	492.330	65.680	315.560	551.714	-57.636
600	454.766	701.559	520.768	108.475	310.798	599.416	-52.183
700	499.089	775.118	551.903	156.250	307.259	647.819	-48.340
800	534.772	844.174	584.168	208.005	304.797	696.643	-45.485
900	563.949	908.901	616.692	262.989	303.271	745.714	-43.279
1000	588.118	969.609	648.980	320.629	302.550	794.920	-41.522
1100	608.343	1026.639	680.747	380.481	302.483	844.172	-40.086
1200	625.404	1080.324	711.831	442.192	302.957	893.393	-38.888
1300	639.895	1130.971	742.143	505.476	303.834	942.564	-37.872
1400	652.276	1178.857	771.642	570.101	305.014	991.660	-36.999
1500	662.914	1224.231	800.316	635.874	306.433	1040.663	-36.238
1600	672.101	1267.315	828.168	702.635	307.994	1089.560	-35.570
1700	680.076	1308.306	855.216	770.253	309.640	1138.339	-34.976
1800	687.030	1347.379	881.481	838.616	311.316	1187.066	-34.447
1900	693.122	1384.692	906.991	907.631	312.997	1235.662	-33.970
2000	698.483	1420.383	931.775	977.216	314.642	1284.189	-33.539
2100	703.219	1454.580	955.862	1047.306	316.195	1332.625	-33.147
2200	707.421	1487.392	979.282	1117.843	317.654	1380.993	-32.788
2300	711.163	1518.922	1002.064	1188.775	319.014	1429.294	-32.460
2400	714.507	1549.261	1024.235	1260.062	320.224	1477.506	-32.156
2500	717.506	1578.491	1045.825	1331.665	321.293	1525.751	-31.878
2600	720.205	1606.685	1066.857	1403.553	322.193	1573.873	-31.619
2700	722.641	1633.913	1087.358	1475.698	322.927	1622.014	-31.379
2800	724.847	1660.234	1107.350	1548.074	323.477	1670.149	-31.156
2900	726.849	1685.705	1126.857	1620.660	323.822	1718.228	-30.948
3000	728.672	1710.378	1145.898	1693.438	323.991	1766.317	-30.754
3100	730.336	1734.298	1164.495	1766.389	323.931	1814.351	-30.571
3200	731.858	1757.510	1182.666	1839.500	323.669	1862.441	-30.401
3300	733.254	1780.052	1200.429	1912.757	323.194	1910.570	-30.241
3400	734.538	1801.961	1217.800	1986.147	322.486	1958.657	-30.090
3500	735.720	1823.271	1234.796	2059.661	321.546	2006.755	-29.949
3600	736.811	1844.012	1251.432	2133.288	320.391	2054.943	-29.816
3700	737.820	1864.214	1267.722	2207.020	319.000	2103.180	-29.691
3800	738.755	1883.903	1283.679	2280.850	317.351	2151.414	-29.573
3900	739.623	1903.104	1299.317	2354.769	315.475	2199.660	-29.461
4000	740.430	1921.840	1314.647	2428.772	313.360	2248.054	-29.356
4100	741.181	1940.132	1329.680	2502.853	310.981	2296.451	-29.257
4200	741.882	1958.001	1344.428	2577.007	308.358	2344.903	-29.163
4300	742.537	1975.466	1358.901	2651.228	305.479	2393.357	-29.073
4400	743.149	1992.544	1373.109	2725.512	302.353	2441.947	-28.989
4500	743.723	2009.251	1387.061	2799.856	298.988	2490.651	-28.910
4600	744.261	2025.603	1400.765	2874.256	295.348	2539.435	-28.836
4700	744.767	2041.615	1414.230	2948.707	291.444	2588.223	-28.764
4800	745.242	2057.300	1427.465	3023.208	287.309	2637.170	-28.698
4900	745.690	2072.671	1440.476	3097.755	282.889	2686.111	-28.634
5000	746.111	2087.740	1453.271	3172.345	278.253	2735.278	-28.575

3.52. 4*H*-Cyclopenta[*def*]chrysene



Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 202-98-2
Point Group: C_s

Length: 13.58 Å
Width: 8.746 Å
Breadth: 4.178 Å
L/B Ratio: 1.552

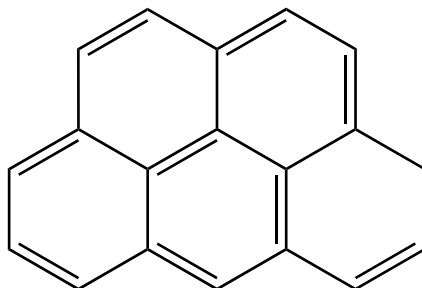
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C	-1.4423	2.2896	0.0000	C	0.5768	-0.8479	0.0000	H	-5.5086	-0.2771	-0.0000
C	-2.4540	1.1566	0.0000	C	1.1995	1.9810	0.0000	H	-4.1952	-2.3682	-0.0000
C	-3.8214	1.0698	-0.0000	C	2.2354	0.9719	-0.0000	H	-1.6922	-3.4454	0.0000
C	-4.4141	-0.2230	-0.0000	C	1.9524	-0.4182	0.0000	H	0.7452	-3.0170	0.0000
C	-3.6893	-1.3974	-0.0000	C	3.0160	-1.3453	0.0000	H	1.4878	3.0373	-0.0000
C	-1.7384	-0.0671	0.0000	C	4.3208	-0.9123	0.0000	H	2.7807	-2.4172	0.0000
C	-2.2717	-1.3470	0.0000	C	4.6078	0.4638	-0.0000	H	5.1439	-1.6342	0.0000
C	-1.3143	-2.4172	0.0000	C	3.5879	1.3859	-0.0000	H	5.6515	0.7946	-0.0000
C	0.0374	-2.1786	0.0000	H	-1.5588	2.9344	-0.8893	H	3.8156	2.4583	-0.0000
C	-0.0971	1.5823	0.0000	H	-1.5588	2.9344	0.8893				
C	-0.3462	0.1726	0.0000	H	-4.4582	1.9590	-0.0000				

Table 3.52: Table of thermodynamic data as a function of temperature for 4*H*-Cyclopenta[*def*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-35.564	314.606	314.606	∞
100	76.706	304.796	610.205	-30.541	335.703	367.468	-191.942
200	152.512	379.833	476.247	-19.283	324.603	403.642	-105.418
250	197.164	418.620	460.821	-10.550	319.335	424.012	-88.591
298.15	240.993	457.100	457.100	0.000	314.606	444.612	-77.893
300	242.661	458.596	457.105	0.447	314.432	445.418	-77.552
350	286.623	499.335	460.222	13.690	310.031	467.606	-69.785
400	327.527	540.318	467.672	29.058	306.170	490.380	-64.036
450	364.672	581.078	478.013	46.379	302.793	513.612	-59.617
500	397.944	621.255	490.334	65.461	299.840	537.212	-56.121
600	453.903	698.955	518.684	108.162	294.986	585.166	-50.942
700	498.340	772.389	549.736	155.858	291.366	633.837	-47.296
800	534.119	841.352	581.924	207.543	288.834	682.938	-44.590
900	563.377	906.007	614.380	262.465	287.247	732.295	-42.500
1000	587.614	966.658	646.607	320.051	286.473	781.794	-40.836
1100	607.895	1023.643	678.319	379.856	286.358	831.343	-39.476
1200	625.005	1077.291	709.353	441.525	286.789	880.865	-38.342
1300	639.537	1127.907	739.622	504.771	287.629	930.342	-37.381
1400	651.954	1175.768	769.081	569.362	288.775	979.745	-36.554
1500	662.623	1221.121	797.719	635.104	290.163	1029.058	-35.834
1600	671.837	1264.187	825.539	701.838	291.696	1078.267	-35.201
1700	679.835	1305.163	852.556	769.431	293.317	1127.360	-34.639
1800	686.810	1344.223	878.795	837.771	294.970	1176.402	-34.138
1900	692.921	1381.524	904.280	906.764	296.630	1225.314	-33.686
2000	698.297	1417.206	929.041	976.330	298.256	1274.158	-33.277
2100	703.048	1451.393	953.106	1046.403	299.791	1322.913	-32.905
2200	707.263	1484.198	976.506	1116.922	301.234	1371.599	-32.565
2300	711.017	1515.722	999.270	1187.840	302.578	1420.220	-32.254
2400	714.371	1546.055	1021.424	1259.112	303.775	1468.753	-31.966
2500	717.380	1575.279	1042.998	1330.703	304.830	1517.318	-31.702
2600	720.087	1603.469	1064.015	1402.578	305.718	1565.762	-31.456
2700	722.531	1630.692	1084.502	1474.711	306.441	1614.225	-31.228
2800	724.743	1657.009	1104.481	1547.077	306.980	1662.682	-31.017
2900	726.752	1682.477	1123.976	1619.653	307.315	1711.084	-30.819
3000	728.581	1707.146	1143.006	1692.421	307.475	1759.496	-30.635
3100	730.250	1731.064	1161.591	1765.364	307.406	1807.853	-30.461
3200	731.777	1754.273	1179.752	1838.466	307.136	1856.267	-30.300
3300	733.178	1776.812	1197.505	1911.715	306.653	1904.719	-30.149
3400	734.465	1798.719	1214.867	1985.098	305.937	1953.130	-30.006
3500	735.651	1820.027	1231.854	2058.605	304.990	2001.552	-29.871
3600	736.746	1840.766	1248.482	2132.225	303.829	2050.065	-29.745
3700	737.758	1860.967	1264.763	2205.951	302.431	2098.627	-29.627
3800	738.696	1880.654	1280.713	2279.775	300.776	2147.185	-29.515
3900	739.567	1899.853	1296.343	2353.688	298.895	2195.756	-29.408
4000	740.376	1918.588	1311.666	2427.686	296.774	2244.475	-29.309
4100	741.130	1936.879	1326.693	2501.762	294.390	2293.198	-29.215
4200	741.833	1954.747	1341.435	2575.910	291.762	2341.975	-29.126
4300	742.490	1972.210	1355.902	2650.127	288.878	2390.755	-29.041
4400	743.105	1989.287	1370.104	2724.407	285.747	2439.670	-28.962
4500	743.680	2005.993	1384.050	2798.746	282.378	2488.700	-28.887
4600	744.220	2022.345	1397.748	2873.142	278.734	2537.810	-28.817
4700	744.727	2038.355	1411.209	2947.589	274.826	2586.923	-28.750
4800	745.204	2054.039	1424.438	3022.086	270.687	2636.197	-28.687
4900	745.653	2069.410	1437.445	3096.629	266.264	2685.464	-28.627
5000	746.077	2084.478	1450.235	3171.216	261.624	2734.958	-28.571

3.53. 3*H*-Benzo[*cd*]pyrene



Other names: 1,10-(peri)-Benzo-1,5-dihydropyrene
1,9,8-(diperi)-Naphth-2,9-dihydroanthracene
peri-Pyrene-1,10(CH₂)-indene

Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 191-35-5
Point Group: C_s

Length: 11.63 Å
Width: 9.523 Å
Breadth: 4.169 Å
L/B Ratio: 1.221

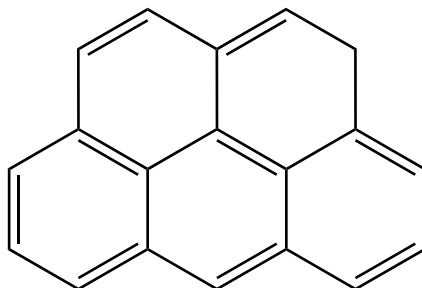
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C	-2.4502	-2.2584	0.0000	C	2.4731	0.6121	0.0000	H	0.0327	-3.3189	0.0000
C	-1.1773	-1.5521	0.0000	C	2.4377	2.0527	0.0000	H	1.2377	3.8186	0.0000
C	-1.2096	-0.1058	0.0000	C	1.2625	2.7229	0.0000	H	3.3933	2.5894	0.0000
C	-2.4216	0.5962	0.0000	C	1.2604	-1.5157	0.0000	H	-3.3645	2.5357	0.0000
C	-3.7275	-0.1249	0.0000	C	0.0074	-2.2223	0.0000	H	-1.2292	3.7949	0.0000
C	-3.6173	-1.6049	0.0000	C	2.4837	-2.1937	0.0000	H	-2.4145	-3.3543	0.0000
C	0.0100	0.6079	0.0000	C	3.6781	-1.4832	0.0000	H	-4.5656	-2.1545	0.0000
C	0.0051	2.0198	0.0000	C	3.6803	-0.0933	0.0000	H	-4.3177	0.1906	-0.8858
C	-1.2182	2.6991	0.0000	H	4.6291	0.4548	0.0000	H	-4.3177	0.1906	0.8858
C	-2.4121	1.9935	0.0000	H	4.6297	-2.0253	0.0000				
C	1.2539	-0.1021	0.0000	H	2.4965	-3.2894	0.0000				

Table 3.53: Table of thermodynamic data as a function of temperature for 3*H*-Benzo[*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-35.354	291.910	291.910	∞
100	75.135	302.734	606.893	-30.416	313.131	345.103	-180.259
200	152.171	377.086	473.329	-19.249	301.940	381.529	-99.643
250	196.852	415.807	457.931	-10.531	296.658	402.038	-83.999
298.15	240.480	454.217	454.217	0.000	291.910	422.775	-74.067
300	242.139	455.709	454.221	0.446	291.734	423.586	-73.751
350	285.854	496.349	457.331	13.656	287.301	445.921	-66.549
400	326.568	537.216	464.763	28.981	283.396	468.847	-61.224
450	363.602	577.856	475.075	46.252	279.969	492.238	-57.136
500	396.834	617.918	487.362	65.278	276.961	516.002	-53.905
600	452.858	695.419	515.634	107.871	271.998	564.300	-49.126
700	497.453	768.703	546.605	155.469	268.281	613.332	-45.766
800	533.411	837.559	578.716	207.074	265.669	662.808	-43.276
900	562.832	902.141	611.103	261.934	264.020	712.548	-41.354
1000	587.205	962.741	643.268	319.473	263.198	762.436	-39.825
1100	607.596	1019.692	674.927	379.243	263.048	812.378	-38.576
1200	624.789	1073.318	705.913	440.886	263.454	862.297	-37.534
1300	639.386	1123.920	736.140	504.114	264.275	912.172	-36.651
1400	651.852	1171.772	765.563	568.692	265.409	961.974	-35.891
1500	662.557	1217.119	794.169	634.426	266.789	1011.687	-35.229
1600	671.799	1260.182	821.960	701.155	268.317	1061.296	-34.647
1700	679.817	1301.156	848.953	768.745	269.935	1110.789	-34.130
1800	686.807	1340.215	875.169	837.084	271.587	1160.232	-33.668
1900	692.929	1377.517	900.634	906.077	273.247	1209.545	-33.252
2000	698.314	1413.199	925.376	975.645	274.874	1258.790	-32.876
2100	703.071	1447.387	949.426	1045.719	276.411	1307.945	-32.533
2200	707.290	1480.193	972.811	1116.241	277.856	1357.032	-32.219
2300	711.046	1511.718	995.561	1187.162	279.204	1406.054	-31.932
2400	714.403	1542.052	1017.703	1258.437	280.403	1454.987	-31.666
2500	717.413	1571.278	1039.265	1330.031	281.462	1503.952	-31.423
2600	720.121	1599.469	1060.273	1401.910	282.353	1552.796	-31.195
2700	722.565	1626.693	1080.750	1474.046	283.079	1601.659	-30.985
2800	724.777	1653.012	1100.721	1546.415	283.622	1650.516	-30.790
2900	726.785	1678.481	1120.207	1618.995	283.960	1699.317	-30.607
3000	728.613	1703.151	1139.229	1691.766	284.123	1748.129	-30.437
3100	730.282	1727.070	1157.808	1764.712	284.057	1796.886	-30.277
3200	731.808	1750.280	1175.962	1837.818	283.791	1845.699	-30.127
3300	733.208	1772.820	1193.708	1911.069	283.310	1894.550	-29.988
3400	734.495	1794.728	1211.065	1984.456	282.598	1943.361	-29.855
3500	735.680	1816.037	1228.047	2057.965	281.654	1992.182	-29.731
3600	736.774	1836.777	1244.669	2131.589	280.495	2041.093	-29.615
3700	737.785	1856.978	1260.946	2205.317	279.100	2090.054	-29.506
3800	738.722	1876.666	1276.891	2279.143	277.448	2139.011	-29.402
3900	739.592	1895.866	1292.517	2353.059	275.569	2187.981	-29.304
4000	740.401	1914.601	1307.836	2427.059	273.451	2237.099	-29.213
4100	741.154	1932.893	1322.859	2501.138	271.070	2286.220	-29.126
4200	741.856	1950.761	1337.598	2575.289	268.444	2335.396	-29.044
4300	742.512	1968.226	1352.061	2649.507	265.562	2384.574	-28.966
4400	743.126	1985.303	1366.260	2723.790	262.434	2433.888	-28.893
4500	743.701	2002.009	1380.202	2798.131	259.066	2483.316	-28.825
4600	744.240	2018.361	1393.898	2872.529	255.425	2532.825	-28.761
4700	744.747	2034.372	1407.356	2946.978	251.518	2582.336	-28.699
4800	745.223	2050.057	1420.582	3021.477	247.381	2632.008	-28.641
4900	745.672	2065.427	1433.586	3096.022	242.960	2681.673	-28.586
5000	746.094	2080.496	1446.374	3170.611	238.321	2731.565	-28.536

3.54. 2H-Benzo[cd]pyrene



Other names: Naphthanthrene

Formula: C₁₉H₁₂

Mass: 240.299 g/mol

CAS Number: 191-32-2

Point Group: C_s

Length: 11.61 Å

Width: 9.551 Å

Breadth: 4.169 Å

L/B Ratio: 1.216

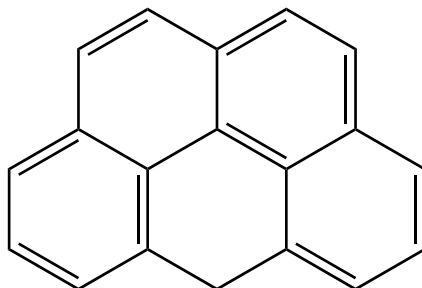
Cartesian coordinates:

C	-1.1853	-2.7054	0.0000	C	2.4983	2.2109	-0.0000	H	0.0420	3.3351	0.0000
C	-0.0173	-2.0308	0.0000	C	3.6645	1.5047	-0.0000	H	-2.4103	3.3640	0.0000
C	0.0007	-0.5744	0.0000	C	3.6565	0.0858	0.0000	H	-4.5674	2.1289	0.0000
C	-1.2098	0.1373	0.0000	C	-1.1896	1.5588	0.0000	H	-4.6029	-0.3440	-0.0000
C	-2.4706	-0.5473	0.0000	C	0.0303	2.2383	0.0000	H	1.2424	-3.8196	0.0000
C	-2.5084	-2.0392	-0.0000	C	-3.6351	0.1695	0.0000	H	3.3867	-2.5861	0.0000
C	1.2253	0.1143	0.0000	C	-3.6136	1.5912	0.0000	H	-3.0803	-2.3894	-0.8854
C	2.4695	-0.6021	0.0000	C	-2.4337	2.2686	0.0000	H	-3.0803	-2.3894	0.8854
C	2.4282	-2.0541	0.0000	H	4.6115	-0.4514	-0.0000	H	-1.1966	-3.8023	-0.0000
C	1.2633	-2.7235	0.0000	H	4.6289	2.0235	-0.0000				
C	1.2388	1.5336	0.0000	H	2.5030	3.3068	-0.0000				

Table 3.54: Table of thermodynamic data as a function of temperature for 2*H*-Benzo[*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-35.603	351.887	351.887	∞
100	75.850	304.008	610.201	-30.619	372.905	404.749	-211.415
200	153.210	378.989	475.788	-19.360	361.807	441.015	-115.179
250	197.991	417.953	460.303	-10.587	356.579	461.422	-96.407
298.15	241.680	456.569	456.569	0.000	351.887	482.051	-84.452
300	243.340	458.070	456.574	0.449	351.714	482.858	-84.071
350	287.065	498.896	459.699	13.719	347.341	505.070	-75.376
400	327.744	539.923	467.163	29.104	343.496	527.864	-68.931
450	364.715	580.697	477.517	46.431	340.126	551.116	-63.971
500	397.871	620.873	489.850	65.512	337.172	574.735	-60.041
600	453.736	698.549	518.215	108.200	332.304	622.729	-54.212
700	498.185	771.957	549.274	155.879	328.668	671.441	-50.102
800	534.021	840.903	581.464	207.551	326.123	720.587	-47.049
900	563.343	905.550	613.921	262.466	324.530	769.989	-44.688
1000	587.636	966.200	646.148	320.052	323.755	819.533	-42.807
1100	607.962	1023.190	677.861	379.862	323.644	869.128	-41.271
1200	625.104	1076.845	708.896	441.539	324.084	918.695	-39.989
1300	639.657	1127.470	739.165	504.796	324.935	968.216	-38.903
1400	652.088	1175.341	768.626	569.400	326.094	1017.662	-37.969
1500	662.765	1220.703	797.266	635.156	327.496	1067.018	-37.156
1600	671.983	1263.779	825.088	701.904	329.043	1116.268	-36.442
1700	679.981	1304.763	852.109	769.512	330.679	1165.401	-35.808
1800	686.953	1343.831	878.350	837.866	332.346	1214.483	-35.243
1900	693.061	1381.140	903.838	906.873	334.021	1263.434	-34.734
2000	698.433	1416.829	928.602	976.454	335.660	1312.316	-34.273
2100	703.179	1451.023	952.671	1046.539	337.208	1361.108	-33.855
2200	707.389	1483.834	976.074	1117.072	338.664	1409.831	-33.473
2300	711.137	1515.363	998.840	1188.002	340.021	1458.488	-33.123
2400	714.486	1545.701	1020.998	1259.286	341.229	1507.056	-32.800
2500	717.489	1574.929	1042.574	1330.887	342.295	1555.657	-32.503
2600	720.191	1603.123	1063.595	1402.774	343.194	1604.136	-32.227
2700	722.630	1630.350	1084.085	1474.917	343.927	1652.633	-31.971
2800	724.838	1656.671	1104.067	1547.292	344.476	1701.124	-31.734
2900	726.842	1682.142	1123.564	1619.878	344.820	1749.559	-31.512
3000	728.667	1706.814	1142.596	1692.654	344.989	1798.005	-31.305
3100	730.332	1730.735	1161.185	1765.606	344.928	1846.395	-31.111
3200	731.855	1753.946	1179.347	1838.716	344.666	1894.841	-30.929
3300	733.252	1776.488	1197.103	1911.972	344.191	1943.327	-30.760
3400	734.536	1798.397	1214.467	1985.363	343.482	1991.770	-30.599
3500	735.719	1819.707	1231.457	2058.876	342.542	2040.224	-30.448
3600	736.811	1840.448	1248.086	2132.503	341.388	2088.768	-30.307
3700	737.820	1860.650	1264.370	2206.236	339.996	2137.362	-30.174
3800	738.755	1880.339	1280.322	2280.065	338.347	2185.952	-30.047
3900	739.624	1899.540	1295.954	2353.984	336.472	2234.555	-29.928
4000	740.431	1918.276	1311.279	2427.988	334.357	2283.305	-29.816
4100	741.182	1936.569	1326.308	2502.069	331.978	2332.058	-29.710
4200	741.883	1954.438	1341.051	2576.222	329.355	2380.867	-29.610
4300	742.538	1971.902	1355.520	2650.444	326.476	2429.678	-29.514
4400	743.151	1988.980	1369.724	2724.729	323.350	2478.624	-29.424
4500	743.725	2005.687	1383.671	2799.073	319.985	2527.684	-29.340
4600	744.263	2022.040	1397.372	2873.472	316.346	2576.825	-29.260
4700	744.769	2038.051	1410.833	2947.924	312.441	2625.968	-29.184
4800	745.244	2053.736	1424.064	3022.425	308.306	2675.272	-29.112
4900	745.692	2069.107	1437.072	3096.972	303.887	2724.569	-29.044
5000	746.114	2084.177	1449.864	3171.563	299.251	2774.093	-28.980

3.55. 6H-Benzo[cd]pyrene



Other names: 1,8,9-Naphthanthrene

Formula: C₁₉H₁₂

Mass: 240.299 g/mol

CAS Number: 191-33-3

Point Group: C_{2v}

Length: 11.66 Å

Width: 9.494 Å

Breadth: 4.171 Å

L/B Ratio: 1.228

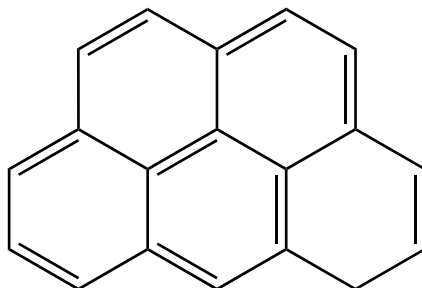
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C	3.6786	0.0874	0.0000	C	-3.6810	1.4766	0.0000	H	1.2102	-3.8094	-0.0000
C	3.6870	1.4616	0.0000	C	-3.6782	0.1024	0.0000	H	3.3722	-2.5861	0.0000
C	2.4801	2.1820	0.0000	C	1.2414	0.1062	0.0000	H	-3.3828	-2.5722	0.0000
C	2.4512	-0.6135	0.0000	C	1.2665	1.5227	0.0000	H	-1.2258	-3.8044	-0.0000
C	1.2363	-2.7137	0.0000	C	0.0047	2.3186	-0.0000	H	-2.4955	3.2876	0.0000
C	2.4195	-2.0443	0.0000	C	-1.2603	1.5279	0.0000	H	-4.6271	2.0279	0.0000
C	-0.0041	-2.0028	0.0000	C	-1.2410	0.1112	0.0000	H	-4.6192	-0.4590	0.0000
C	-2.4278	-2.0344	0.0000	C	-0.0012	-0.6090	0.0000	H	0.0061	2.9885	0.8856
C	-1.2474	-2.7086	0.0000	H	4.6172	-0.4780	0.0000	H	0.0061	2.9885	-0.8856
C	-2.4537	-0.6035	0.0000	H	4.6353	2.0091	0.0000				
C	-2.4712	2.1921	0.0000	H	2.5090	3.2774	0.0000				

Table 3.55: Table of thermodynamic data as a function of temperature for 6*H*-Benzo[*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-35.450	272.474	272.474	∞
100	75.713	304.179	607.365	-30.319	293.792	325.619	-170.083
200	151.508	378.501	474.316	-19.163	282.590	361.896	-94.515
250	195.946	417.043	458.985	-10.486	277.267	382.338	-79.883
298.15	239.527	455.287	455.287	0.000	272.474	403.020	-70.606
300	241.186	456.774	455.292	0.445	272.296	403.829	-70.311
350	284.972	497.272	458.390	13.608	267.817	426.114	-63.593
400	325.805	538.028	465.798	28.892	263.871	448.997	-58.632
450	362.966	578.585	476.080	46.127	260.408	472.349	-54.828
500	396.313	618.587	488.336	65.125	257.372	496.079	-51.824
600	452.503	696.008	516.550	107.675	252.365	544.314	-47.386
700	497.193	769.246	547.471	155.243	248.618	593.289	-44.271
800	533.199	838.071	579.540	206.825	245.983	642.713	-41.964
900	562.645	902.629	611.890	261.665	244.314	692.403	-40.185
1000	587.032	963.211	644.025	319.186	243.474	742.243	-38.770
1100	607.431	1020.146	675.656	378.938	243.307	792.139	-37.615
1200	624.632	1073.757	706.619	440.565	243.697	842.013	-36.651
1300	639.235	1124.347	736.825	503.778	244.503	891.845	-35.834
1400	651.708	1172.188	766.229	568.342	245.622	941.605	-35.131
1500	662.421	1217.525	794.818	634.061	246.988	991.277	-34.519
1600	671.670	1260.579	822.594	700.777	248.503	1040.846	-33.979
1700	679.695	1301.546	849.572	768.355	250.108	1090.300	-33.500
1800	686.692	1340.598	875.775	836.682	251.749	1139.704	-33.073
1900	692.821	1377.894	901.229	905.664	253.398	1188.979	-32.687
2000	698.212	1413.571	925.960	975.221	255.014	1238.186	-32.337
2100	702.975	1447.754	949.999	1045.286	256.541	1287.305	-32.019
2200	707.200	1480.556	973.375	1115.798	257.977	1336.355	-31.728
2300	710.961	1512.077	996.116	1186.710	259.316	1385.341	-31.461
2400	714.323	1542.408	1018.250	1257.977	260.507	1434.238	-31.215
2500	717.337	1571.630	1039.805	1329.563	261.558	1483.168	-30.988
2600	720.049	1599.818	1060.805	1401.435	262.441	1531.977	-30.777
2700	722.497	1627.040	1081.275	1473.564	263.161	1580.805	-30.582
2800	724.713	1653.356	1101.239	1545.926	263.697	1629.627	-30.400
2900	726.725	1678.823	1120.719	1618.500	264.029	1678.394	-30.231
3000	728.556	1703.491	1139.736	1691.265	264.186	1727.172	-30.072
3100	730.228	1727.408	1158.309	1764.206	264.115	1775.895	-29.923
3200	731.757	1750.616	1176.458	1837.306	263.843	1824.674	-29.784
3300	733.159	1773.155	1194.200	1910.553	263.358	1873.492	-29.654
3400	734.448	1795.062	1211.552	1983.934	262.640	1922.269	-29.531
3500	735.636	1816.369	1228.529	2057.439	261.692	1971.057	-29.416
3600	736.732	1837.108	1245.148	2131.058	260.529	2019.935	-29.308
3700	737.745	1857.308	1261.421	2204.783	259.130	2068.863	-29.207
3800	738.684	1876.995	1277.362	2278.605	257.474	2117.787	-29.110
3900	739.556	1896.194	1292.984	2352.517	255.591	2166.724	-29.019
4000	740.366	1914.928	1308.300	2426.514	253.470	2215.809	-28.935
4100	741.120	1933.219	1323.319	2500.589	251.085	2264.897	-28.855
4200	741.824	1951.087	1338.054	2574.736	248.455	2314.041	-28.779
4300	742.482	1968.550	1352.515	2648.952	245.571	2363.187	-28.706
4400	743.097	1985.627	1366.710	2723.231	242.439	2412.468	-28.639
4500	743.673	2002.333	1380.650	2797.570	239.069	2461.864	-28.576
4600	744.213	2018.684	1394.344	2871.965	235.424	2511.340	-28.517
4700	744.721	2034.694	1407.798	2946.412	231.515	2560.819	-28.460
4800	745.198	2050.378	1421.023	3020.908	227.376	2610.459	-28.407
4900	745.647	2065.748	1434.024	3095.450	222.952	2660.092	-28.356
5000	746.071	2080.817	1446.810	3170.036	218.311	2709.952	-28.310

3.56. 5H-Benzo[cd]pyrene



Other names: Pyrenindene
Formula: C₁₉H₁₂
Mass: 240.299 g/mol
CAS Number: 191-34-4
Point Group: C_s

Length: 11.83 Å
Width: 9.618 Å
Breadth: 4.170 Å
L/B Ratio: 1.230

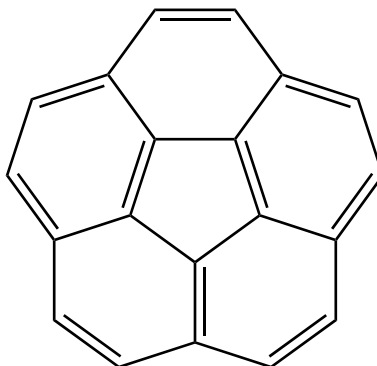
Cartesian coordinates:

C	-3.6756	-0.1365	0.0000	C	2.3903	2.0368	0.0000	H	0.0181	-3.3079	0.0000
C	-3.6536	-1.5260	0.0000	C	1.1859	2.7229	0.0000	H	-1.2838	3.8076	-0.0000
C	-2.4492	-2.2200	0.0000	C	1.2130	-0.0855	0.0000	H	-3.4237	2.5512	0.0000
C	-1.2360	-1.5246	0.0000	C	1.2047	-1.5298	0.0000	H	3.3349	2.5930	0.0000
C	0.0283	-2.2112	0.0000	C	2.5006	-2.2723	0.0000	H	1.1791	3.8188	0.0000
C	-2.4785	0.5860	0.0000	C	3.7152	-1.4202	0.0000	H	2.5374	-2.9412	0.8855
C	-1.2499	-0.1117	0.0000	C	3.6779	-0.0824	0.0000	H	2.5374	-2.9412	-0.8855
C	-1.2943	2.7116	0.0000	C	2.4162	0.6380	0.0000	H	4.6728	-1.9534	0.0000
C	-2.4614	2.0266	0.0000	H	-4.6321	0.3983	0.0000	H	4.5983	0.5130	0.0000
C	-0.0281	2.0253	0.0000	H	-4.5973	-2.0817	0.0000				
C	-0.0152	0.6131	0.0000	H	-2.4468	-3.3157	0.0000				

Table 3.56: Table of thermodynamic data as a function of temperature for 5*H*-Benzo[*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-35.455	297.354	297.354	∞
100	75.644	304.205	608.760	-30.455	318.536	350.360	-183.006
200	152.323	378.777	475.070	-19.259	307.375	386.625	-100.974
250	196.946	417.525	459.664	-10.535	302.099	407.049	-85.046
298.15	240.555	455.949	455.949	0.000	297.354	427.703	-74.930
300	242.213	457.442	455.954	0.447	297.179	428.511	-74.609
350	285.929	498.094	459.064	13.660	292.750	450.759	-67.271
400	326.648	538.971	466.498	28.989	288.848	473.597	-61.844
450	363.688	579.620	476.813	46.263	285.425	496.900	-57.677
500	396.924	619.692	489.103	65.294	282.422	520.576	-54.383
600	452.946	697.209	517.382	107.896	277.467	568.696	-49.508
700	497.531	770.506	548.360	155.503	273.759	617.548	-46.081
800	533.476	839.372	580.478	207.115	271.155	666.843	-43.539
900	562.884	903.960	612.870	261.981	269.511	716.402	-41.578
1000	587.245	964.566	645.041	319.524	268.694	766.107	-40.016
1100	607.626	1021.520	676.704	379.297	268.547	815.867	-38.741
1200	624.813	1075.148	707.695	440.943	268.956	865.603	-37.678
1300	639.403	1125.751	737.926	504.173	269.779	915.294	-36.776
1400	651.864	1173.604	767.352	568.753	270.914	964.913	-36.001
1500	662.566	1218.952	795.961	634.488	272.295	1014.443	-35.325
1600	671.805	1262.016	823.755	701.217	273.824	1063.869	-34.731
1700	679.822	1302.990	850.750	768.808	275.442	1113.179	-34.203
1800	686.810	1342.050	876.968	837.147	277.095	1162.438	-33.732
1900	692.931	1379.351	902.435	906.141	278.756	1211.568	-33.308
2000	698.315	1415.034	927.179	975.709	280.383	1260.629	-32.924
2100	703.071	1449.222	951.230	1045.783	281.920	1309.601	-32.574
2200	707.290	1482.028	974.616	1116.305	283.365	1358.505	-32.254
2300	711.046	1513.553	997.368	1187.226	284.712	1407.343	-31.961
2400	714.402	1543.887	1019.511	1258.501	285.912	1456.092	-31.690
2500	717.412	1573.112	1041.074	1330.095	286.970	1504.874	-31.442
2600	720.119	1601.303	1062.083	1401.973	287.861	1553.535	-31.210
2700	722.563	1628.527	1082.561	1474.110	288.587	1602.214	-30.996
2800	724.775	1654.846	1102.532	1546.478	289.130	1650.887	-30.797
2900	726.784	1680.315	1122.019	1619.058	289.467	1699.506	-30.611
3000	728.612	1704.985	1141.042	1691.829	289.631	1748.134	-30.437
3100	730.280	1728.904	1159.622	1764.775	289.564	1796.707	-30.274
3200	731.807	1752.114	1177.776	1837.880	289.298	1845.337	-30.121
3300	733.207	1774.655	1195.524	1911.132	288.817	1894.005	-29.979
3400	734.493	1796.562	1212.881	1984.518	288.104	1942.632	-29.844
3500	735.678	1817.871	1229.863	2058.027	287.161	1991.270	-29.717
3600	736.772	1838.611	1246.486	2131.651	286.002	2039.998	-29.599
3700	737.784	1858.812	1262.763	2205.379	284.606	2088.775	-29.488
3800	738.721	1878.500	1278.709	2279.205	282.954	2137.549	-29.382
3900	739.591	1897.700	1294.335	2353.121	281.075	2186.335	-29.282
4000	740.399	1916.435	1309.655	2427.121	278.957	2235.270	-29.189
4100	741.152	1934.727	1324.678	2501.199	276.575	2284.207	-29.101
4200	741.855	1952.595	1339.417	2575.350	273.949	2333.200	-29.017
4300	742.511	1970.059	1353.880	2649.568	271.068	2382.195	-28.937
4400	743.125	1987.136	1368.079	2723.850	267.939	2431.326	-28.863
4500	743.700	2003.843	1382.022	2798.192	264.571	2480.570	-28.793
4600	744.239	2020.195	1395.719	2872.589	260.930	2529.896	-28.727
4700	744.746	2036.206	1409.176	2947.039	257.023	2579.224	-28.664
4800	745.222	2051.890	1422.403	3021.537	252.886	2628.712	-28.606
4900	745.671	2067.261	1435.407	3096.082	248.465	2678.194	-28.549
5000	746.093	2082.330	1448.196	3170.671	243.826	2727.902	-28.498

3.57. Dibenzo[*ghi,mno*]fluoranthene



Other names: Corannulene
Formula: $C_{20}H_{10}$
Mass: 250.293 g/mol
CAS Number: 5821-51-2
Point Group: C_{5v}

Length: 10.86 Å
Width: 10.45 Å
Breadth: 4.830 Å
L/B Ratio: 1.039

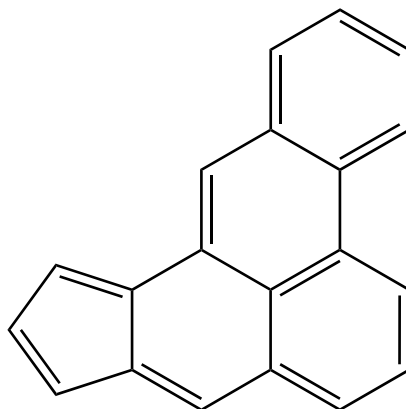
Cartesian coordinates:

C	2.7672	1.6796	-0.3010	C	-1.1514	-0.3960	0.6420	H	1.1642	4.0712	-0.6396
C	1.4172	2.0227	0.0657	C	-2.3354	-0.8033	0.0655	H	-1.3029	4.0290	-0.6397
C	0.6987	0.9972	0.6420	C	-3.2260	0.2679	-0.3008	H	-3.5113	2.3649	-0.6423
C	1.1643	-0.3564	0.6420	C	-2.8233	1.5840	-0.3005	H	-4.2330	0.0054	-0.6431
C	2.3616	-0.7229	0.0657	C	0.0208	-1.2175	0.6422	H	-3.3342	-2.6088	-0.6419
C	3.2149	0.3781	-0.3010	C	0.0424	-2.4696	0.0663	H	-1.3134	-4.0250	-0.6407
C	0.6338	3.1751	-0.2993	C	-1.2517	-2.9857	-0.2997	H	3.4219	-2.4934	-0.6407
C	-0.7423	3.1515	-0.2992	C	-2.3788	-2.1959	-0.3002	H	1.4506	-3.9780	-0.6395
C	-1.4857	1.9730	0.0659	C	2.4528	-2.1133	-0.2996	H	4.2303	0.1505	-0.6434
C	-0.7325	0.9727	0.6420	C	1.3534	-2.9413	-0.2992	H	3.4276	2.4838	-0.6436

Table 3.57: Table of thermodynamic data as a function of temperature for Dibenzo[*ghi,mno*]fluoranthene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-33.784	508.432	508.432	∞
100	67.157	280.895	574.315	-29.342	526.250	550.428	-287.508
200	146.817	350.190	444.633	-18.889	516.713	578.415	-151.063
250	193.333	387.925	429.485	-10.390	512.312	594.351	-124.180
298.15	238.035	425.817	425.817	0.000	508.432	610.514	-106.957
300	239.722	427.295	425.822	0.442	508.289	611.146	-106.408
350	283.881	467.603	428.904	13.544	504.727	628.578	-93.808
400	324.579	508.209	436.279	28.772	501.629	646.481	-84.420
450	361.303	548.599	446.519	45.936	498.928	664.753	-77.161
500	394.038	588.394	458.723	64.836	496.558	683.323	-71.385
600	448.739	665.273	486.798	107.085	492.602	721.065	-62.773
700	491.788	737.809	517.529	154.195	489.563	759.400	-56.666
800	526.127	805.803	549.361	205.154	487.336	798.102	-52.110
900	553.954	869.433	581.428	259.205	485.817	837.034	-48.579
1000	576.815	929.020	613.240	315.779	484.911	876.112	-45.762
1100	595.811	984.914	644.515	374.439	484.496	915.263	-43.461
1200	611.739	1037.459	675.093	434.839	484.486	954.420	-41.544
1300	625.200	1086.971	704.890	496.705	484.767	993.573	-39.921
1400	636.654	1133.733	733.867	559.813	485.255	1032.699	-38.530
1500	646.461	1178.001	762.014	623.981	485.903	1071.786	-37.322
1600	654.906	1219.999	789.337	689.059	486.626	1110.820	-36.264
1700	662.219	1259.927	815.854	754.924	487.381	1149.792	-35.328
1800	668.583	1297.963	841.589	821.472	488.119	1188.764	-34.496
1900	674.148	1334.263	866.572	888.614	488.821	1227.658	-33.750
2000	679.038	1368.970	890.830	956.279	489.456	1266.537	-33.078
2100	683.353	1402.207	914.396	1024.403	489.970	1305.375	-32.469
2200	687.177	1434.086	937.298	1092.933	490.365	1344.193	-31.915
2300	690.579	1464.709	959.568	1161.824	490.641	1382.998	-31.408
2400	693.617	1494.165	981.233	1231.037	490.749	1421.757	-30.943
2500	696.339	1522.536	1002.321	1300.537	490.699	1460.596	-30.517
2600	698.787	1549.896	1022.859	1370.295	490.467	1499.357	-30.122
2700	700.995	1576.310	1042.871	1440.286	490.058	1538.185	-29.757
2800	702.993	1601.840	1062.381	1510.487	489.454	1577.044	-29.420
2900	704.807	1626.541	1081.411	1580.879	488.636	1615.891	-29.105
3000	706.457	1650.464	1099.983	1651.443	487.635	1654.789	-28.812
3100	707.962	1673.653	1118.116	1722.165	486.397	1693.667	-28.538
3200	709.339	1696.152	1135.830	1793.031	484.953	1732.643	-28.282
3300	710.602	1717.999	1153.142	1864.029	483.291	1771.696	-28.043
3400	711.762	1739.230	1170.069	1935.148	481.390	1810.738	-27.818
3500	712.830	1759.878	1186.627	2006.379	479.256	1849.827	-27.607
3600	713.816	1779.973	1202.831	2077.712	476.904	1889.046	-27.409
3700	714.728	1799.544	1218.695	2149.140	474.312	1928.342	-27.223
3800	715.572	1818.616	1234.233	2220.655	471.462	1967.672	-27.047
3900	716.356	1837.213	1249.456	2292.252	468.384	2007.039	-26.881
4000	717.084	1855.359	1264.378	2363.924	465.066	2046.590	-26.725
4100	717.763	1873.074	1279.009	2435.667	461.484	2086.174	-26.578
4200	718.395	1890.378	1293.360	2507.475	457.657	2125.842	-26.438
4300	718.986	1907.289	1307.442	2579.345	453.577	2165.539	-26.306
4400	719.539	1923.825	1321.263	2651.271	449.248	2205.399	-26.181
4500	720.056	1940.001	1334.834	2723.251	444.683	2245.400	-26.063
4600	720.542	1955.832	1348.162	2795.282	439.844	2285.514	-25.952
4700	720.998	1971.333	1361.257	2867.359	434.741	2325.653	-25.846
4800	721.427	1986.517	1374.126	2939.480	429.407	2365.980	-25.747
4900	721.830	2001.397	1386.776	3011.643	423.790	2406.321	-25.651
5000	722.211	2015.984	1399.215	3083.845	417.958	2446.914	-25.562

3.58. Benzo[de]cyclopent[a]anthracene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 198-46-9
Point Group: C_s

Length: 13.19 Å
Width: 10.18 Å
Breadth: 3.884 Å
L/B Ratio: 1.296

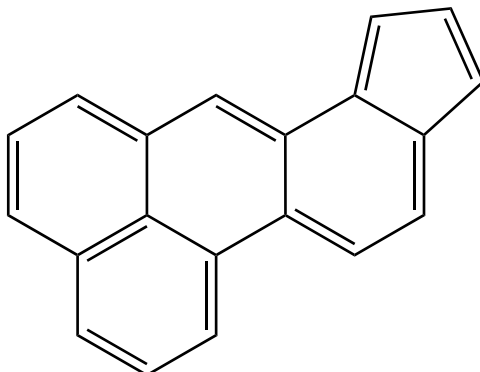
Cartesian coordinates:

C	-4.3355	0.6569	0.0000	C	2.1056	-0.0897	0.0000	H	-2.2296	3.2506	0.0000
C	-3.0330	-0.0180	0.0000	C	1.0662	-1.0968	0.0000	H	-3.4626	-2.1109	0.0000
C	-2.0189	1.0544	0.0000	C	3.4727	-0.4397	0.0000	H	-1.7318	-3.8132	0.0000
C	-2.6683	2.2548	0.0000	C	4.4458	0.5335	0.0000	H	0.6549	-4.4891	0.0000
C	-4.1118	1.9984	0.0000	C	4.0874	1.8917	0.0000	H	2.4494	-2.7592	0.0000
C	-2.7041	-1.3197	0.0000	C	2.7606	2.2568	0.0000	H	0.1172	2.7165	0.0000
C	-1.2994	-1.6999	0.0000	C	-0.9509	-3.0438	0.0000	H	3.7406	-1.5073	0.0000
C	-0.2854	-0.7042	0.0000	C	0.3946	-3.4254	0.0000	H	5.5047	0.2551	0.0000
C	-0.6182	0.7046	0.0000	C	1.3872	-2.4690	0.0000	H	4.8715	2.6559	0.0000
C	0.3676	1.6479	0.0000	H	-4.8581	2.7899	0.0000	H	2.4746	3.3148	0.0000
C	1.7495	1.2704	0.0000	H	-5.2892	0.1345	0.0000				

Table 3.58: Table of thermodynamic data as a function of temperature for Benzo[de]cyclopent[a]anthracene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-38.001	429.798	429.798	∞
100	83.697	313.773	639.786	-32.601	449.825	480.788	-251.133
200	162.824	394.678	497.069	-20.478	439.264	515.951	-134.750
250	209.384	435.969	480.700	-11.183	434.263	535.701	-111.926
298.15	255.022	476.758	476.758	0.000	429.798	555.654	-97.346
300	256.756	478.341	476.763	0.473	429.634	556.434	-96.882
350	302.372	521.381	480.058	14.463	425.509	577.902	-86.245
400	344.656	564.560	487.923	30.655	421.919	599.917	-78.340
450	382.922	607.404	498.824	48.861	418.800	622.358	-72.240
500	417.090	649.553	511.796	68.878	416.085	645.139	-67.396
600	474.329	730.865	541.592	113.564	411.636	691.390	-60.190
700	519.580	807.514	574.164	163.345	408.329	738.297	-55.091
800	555.900	879.350	607.872	217.183	406.029	785.595	-51.293
900	585.541	946.594	641.813	274.303	404.605	833.124	-48.352
1000	610.069	1009.596	675.475	334.121	403.939	880.779	-46.006
1100	630.587	1068.732	708.565	396.184	403.888	928.477	-44.089
1200	647.897	1124.364	740.920	460.132	404.348	976.144	-42.490
1300	662.603	1176.819	772.453	525.676	405.187	1023.764	-41.134
1400	675.175	1226.396	803.123	592.581	406.308	1071.311	-39.970
1500	685.983	1273.356	832.921	660.653	407.651	1118.771	-38.958
1600	695.322	1317.933	861.853	729.729	409.121	1166.130	-38.069
1700	703.433	1360.336	889.938	799.676	410.664	1213.377	-37.282
1800	710.509	1400.748	917.203	870.381	412.225	1260.580	-36.580
1900	716.712	1439.333	943.676	941.749	413.781	1307.657	-35.949
2000	722.172	1476.237	969.388	1013.699	415.291	1354.673	-35.380
2100	726.999	1511.591	994.371	1086.162	416.699	1401.604	-34.862
2200	731.282	1545.512	1018.657	1159.081	418.003	1448.474	-34.390
2300	735.098	1578.105	1042.277	1232.403	419.200	1495.285	-33.958
2400	738.510	1609.464	1065.261	1306.087	420.237	1542.012	-33.560
2500	741.570	1639.674	1087.637	1380.093	421.124	1588.783	-33.195
2600	744.324	1668.814	1109.433	1454.391	421.833	1635.435	-32.856
2700	746.811	1696.952	1130.675	1528.949	422.368	1682.117	-32.542
2800	749.063	1724.153	1151.387	1603.745	422.709	1728.799	-32.250
2900	751.108	1750.475	1171.594	1678.755	422.836	1775.433	-31.978
3000	752.971	1775.971	1191.317	1753.961	422.779	1822.084	-31.725
3100	754.671	1800.689	1210.578	1829.344	422.482	1868.686	-31.486
3200	756.226	1824.673	1229.395	1904.890	421.976	1915.354	-31.264
3300	757.653	1847.966	1247.789	1980.585	421.247	1962.070	-31.056
3400	758.965	1870.604	1265.775	2056.417	420.275	2008.748	-30.860
3500	760.173	1892.622	1283.372	2132.374	419.063	2055.445	-30.675
3600	761.289	1914.053	1300.595	2208.448	417.627	2102.244	-30.502
3700	762.321	1934.925	1317.458	2284.629	415.944	2149.100	-30.339
3800	763.277	1955.268	1333.976	2360.910	413.994	2195.958	-30.185
3900	764.164	1975.106	1350.162	2437.282	411.809	2242.835	-30.039
4000	764.989	1994.464	1366.029	2513.741	409.375	2289.872	-29.902
4100	765.758	2013.363	1381.588	2590.278	406.667	2336.919	-29.772
4200	766.475	2031.824	1396.851	2666.891	403.705	2384.028	-29.649
4300	767.145	2049.868	1411.828	2743.572	400.478	2431.145	-29.532
4400	767.771	2067.511	1426.530	2820.318	396.994	2478.408	-29.422
4500	768.358	2084.772	1440.967	2897.125	393.263	2525.795	-29.318
4600	768.909	2101.666	1455.147	2973.989	389.247	2573.272	-29.220
4700	769.426	2118.208	1469.079	3050.906	384.956	2620.756	-29.126
4800	769.913	2134.412	1482.772	3127.873	380.425	2668.412	-29.038
4900	770.371	2150.292	1496.233	3204.887	375.599	2716.066	-28.953
5000	770.803	2165.860	1509.471	3281.946	370.548	2763.959	-28.874

3.59. Benzo[fg]cyclopent[a]anthracene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 200-63-5
Point Group: C_s

Length: 13.08 Å
Width: 9.172 Å
Breadth: 3.885 Å
L/B Ratio: 1.426

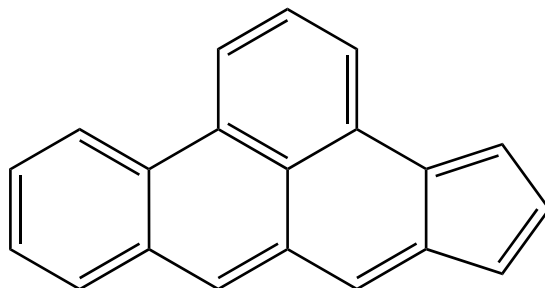
Cartesian coordinates:

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C	0.5318	-0.9097	0.0000	C	-3.4156	2.3481	0.0000	H	0.9264	-3.0051	0.0000
C	1.0667	0.4527	0.0000	C	-2.0159	2.5035	0.0000	H	3.4056	-2.7752	0.0000
C	0.2488	1.5350	0.0000	C	-1.5084	-2.3206	0.0000	H	0.6659	2.5505	0.0000
C	-1.1902	1.3960	0.0000	C	-2.9108	-2.4648	0.0000	H	-1.5869	3.5121	0.0000
C	-1.7555	0.0876	0.0000	C	-3.7235	-1.3626	0.0000	H	-4.0497	3.2411	0.0000
C	2.5042	0.5797	0.0000	C	4.7280	-0.1750	0.0000	H	-5.0687	0.9749	0.0000
C	3.3378	-0.6351	0.0000	C	4.7181	1.1863	0.0000	H	-4.8144	-1.4680	0.0000
C	2.7927	-1.8681	0.0000	C	3.3345	1.6660	0.0000	H	-3.3401	-3.4722	0.0000
C	1.3597	-1.9925	0.0000	H	3.0565	2.7179	0.0000	H	-0.8680	-3.2165	0.0000
C	-3.1583	-0.0592	0.0000	H	5.5883	-0.8401	0.0000				

Table 3.59: Table of thermodynamic data as a function of temperature for Benzo[fg]cyclopent[a]anthracene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-38.365	482.858	482.858	∞
100	84.723	318.932	646.992	-32.806	502.680	533.127	-278.471
200	163.861	400.489	503.432	-20.589	492.214	567.738	-148.275
250	210.526	442.024	486.978	-11.238	487.268	587.192	-122.685
298.15	256.179	483.017	483.017	0.000	482.858	606.848	-106.315
300	257.913	484.607	483.022	0.476	482.696	607.616	-105.793
350	303.492	527.823	486.331	14.522	478.629	628.767	-93.836
400	345.719	571.147	494.226	30.768	475.093	650.456	-84.939
450	383.921	614.114	505.165	49.027	472.025	672.564	-78.068
500	418.026	656.364	518.180	69.092	469.359	695.008	-72.605
600	475.141	737.836	548.061	113.865	464.997	740.569	-64.471
700	520.281	814.601	580.713	163.722	461.766	786.772	-58.708
800	556.505	886.525	614.494	217.625	459.531	833.357	-54.412
900	586.063	953.835	648.500	274.801	458.164	880.165	-51.082
1000	610.522	1016.888	682.220	334.668	457.546	927.094	-48.425
1100	630.981	1076.065	715.363	396.772	457.537	974.061	-46.253
1200	648.242	1131.728	747.764	460.758	458.034	1020.992	-44.442
1300	662.908	1184.210	779.337	526.335	458.905	1067.874	-42.907
1400	675.446	1233.808	810.044	593.268	460.055	1114.681	-41.588
1500	686.224	1280.785	839.875	661.365	461.424	1161.400	-40.443
1600	695.538	1325.378	868.837	730.464	462.917	1208.015	-39.437
1700	703.627	1367.793	896.950	800.432	464.481	1254.517	-38.546
1800	710.685	1408.215	924.240	871.156	466.060	1300.973	-37.752
1900	716.872	1446.809	950.736	942.540	467.633	1347.303	-37.039
2000	722.318	1483.722	976.469	1014.505	469.158	1393.571	-36.396
2100	727.132	1519.082	1001.472	1086.983	470.579	1439.753	-35.811
2200	731.405	1553.009	1025.776	1159.914	471.896	1485.873	-35.278
2300	735.211	1585.607	1049.412	1233.248	473.105	1531.935	-34.791
2400	738.614	1616.971	1072.411	1306.943	474.153	1577.912	-34.342
2500	741.666	1647.185	1094.802	1380.959	475.050	1623.932	-33.929
2600	744.414	1676.328	1116.611	1455.266	475.768	1669.833	-33.547
2700	746.895	1704.470	1137.865	1529.833	476.312	1715.762	-33.193
2800	749.141	1731.674	1158.590	1604.637	476.661	1761.693	-32.864
2900	751.181	1757.999	1178.808	1679.655	476.795	1807.574	-32.557
3000	753.039	1783.497	1198.541	1754.867	476.745	1853.473	-32.271
3100	754.735	1808.217	1217.811	1830.257	476.455	1899.322	-32.003
3200	756.287	1832.204	1236.638	1905.809	475.956	1945.237	-31.752
3300	757.710	1855.498	1255.040	1981.510	475.232	1991.200	-31.517
3400	759.019	1878.137	1273.035	2057.347	474.266	2037.125	-31.296
3500	760.224	1900.157	1290.640	2133.310	473.059	2083.069	-31.087
3600	761.337	1921.589	1307.870	2209.389	471.628	2129.114	-30.892
3700	762.366	1942.463	1324.740	2285.575	469.949	2175.216	-30.708
3800	763.320	1962.807	1341.265	2361.860	468.004	2221.321	-30.534
3900	764.205	1982.646	1357.457	2438.237	465.823	2267.443	-30.368
4000	765.029	2002.005	1373.330	2514.699	463.393	2313.727	-30.214
4100	765.795	2020.905	1388.895	2591.241	460.689	2360.019	-30.066
4200	766.511	2039.367	1404.163	2667.856	457.731	2406.374	-29.927
4300	767.179	2057.412	1419.146	2744.541	454.508	2452.737	-29.794
4400	767.804	2075.056	1433.853	2821.291	451.027	2499.245	-29.669
4500	768.390	2092.317	1448.295	2898.101	447.299	2545.877	-29.551
4600	768.939	2109.212	1462.480	2974.967	443.286	2592.600	-29.439
4700	769.455	2125.754	1476.417	3051.887	438.998	2639.330	-29.332
4800	769.940	2141.959	1490.114	3128.857	434.470	2686.231	-29.232
4900	770.397	2157.839	1503.579	3205.874	429.647	2733.130	-29.135
5000	770.828	2173.408	1516.821	3282.936	424.598	2780.269	-29.045

3.60. Benzo[*de*]cyclopent[*b*]anthracene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 27706-08-7
Point Group: C_s

Length: 13.94 Å
Width: 9.567 Å
Breadth: 3.884 Å
L/B Ratio: 1.457

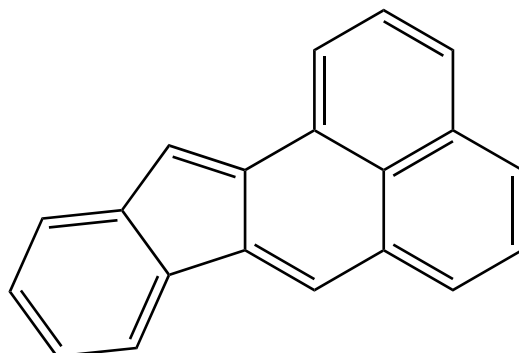
Cartesian coordinates:

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C	0.9431	-1.0056	0.0000	C	-1.4714	1.9184	0.0000	H	-1.4227	3.0135	0.0000
C	-0.2616	-0.2803	0.0000	C	3.4379	-0.9883	0.0000	H	1.0070	2.9208	0.0000
C	-1.4983	-0.9861	0.0000	C	4.6269	-0.2970	0.0000	H	3.4222	-2.0891	0.0000
C	-1.5071	-2.3713	0.0000	C	4.6289	1.1088	0.0000	H	5.5795	-0.8369	0.0000
C	-0.3012	-3.0853	0.0000	C	3.4407	1.8013	0.0000	H	5.5830	1.6460	0.0000
C	-0.2247	1.1647	0.0000	C	-4.0361	-0.5715	0.0000	H	3.4353	2.8973	0.0000
C	0.9717	1.8237	0.0000	C	-4.8450	0.6514	0.0000	H	-2.4602	-2.9127	0.0000
C	2.2099	1.1063	0.0000	C	-4.0272	1.7380	0.0000	H	-0.3236	-4.1801	0.0000
C	2.2049	-0.2998	0.0000	H	-4.3060	2.7890	0.0000	H	1.8544	-2.9683	0.0000
C	-2.7192	-0.2152	0.0000	H	-5.9329	0.6465	0.0000				

Table 3.60: Table of thermodynamic data as a function of temperature for Benzo[de]cyclopent[b]anthracene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-38.018	427.479	427.479	∞
100	83.757	314.077	640.161	-32.608	447.498	478.431	-249.902
200	162.863	395.027	497.422	-20.479	436.944	513.561	-134.126
250	209.392	436.324	481.053	-11.182	431.944	533.294	-111.423
298.15	254.996	477.112	477.112	0.000	427.479	553.229	-96.921
300	256.729	478.694	477.116	0.473	427.314	554.008	-96.459
350	302.313	521.727	480.411	14.461	423.188	575.460	-85.881
400	344.572	564.897	488.275	30.649	419.594	597.457	-78.018
450	382.821	607.730	499.173	48.851	416.470	619.881	-71.952
500	416.979	649.867	512.142	68.862	413.749	642.647	-67.135
600	474.212	731.159	541.932	113.536	409.289	688.867	-59.970
700	519.469	807.790	574.495	163.306	405.971	735.745	-54.901
800	555.798	879.612	608.195	217.133	403.660	783.017	-51.125
900	585.448	946.844	642.129	274.244	402.227	830.520	-48.201
1000	609.986	1009.837	675.784	334.053	401.552	878.151	-45.869
1100	630.512	1068.966	708.868	396.108	401.493	925.825	-43.963
1200	647.830	1124.591	741.217	460.049	401.946	973.469	-42.373
1300	662.543	1177.042	772.744	525.587	402.778	1021.066	-41.026
1400	675.121	1226.614	803.409	592.486	403.893	1068.591	-39.869
1500	685.934	1273.570	833.202	660.552	405.231	1116.030	-38.863
1600	695.278	1318.145	862.130	729.624	406.697	1163.368	-37.979
1700	703.392	1360.545	890.211	799.567	408.236	1210.594	-37.196
1800	710.473	1400.955	917.472	870.268	409.793	1257.776	-36.499
1900	716.678	1439.538	943.942	941.632	411.345	1304.832	-35.872
2000	722.141	1476.440	969.651	1013.579	412.852	1351.827	-35.305
2100	726.970	1511.793	994.631	1086.040	414.256	1398.739	-34.791
2200	731.256	1545.712	1018.915	1158.955	415.558	1445.588	-34.322
2300	735.074	1578.304	1042.532	1232.275	416.752	1492.379	-33.892
2400	738.487	1609.662	1065.513	1305.956	417.787	1539.087	-33.497
2500	741.549	1639.872	1087.887	1379.961	418.672	1585.838	-33.134
2600	744.305	1669.010	1109.681	1454.256	419.379	1632.471	-32.796
2700	746.793	1697.148	1130.921	1528.813	419.912	1679.132	-32.484
2800	749.046	1724.348	1151.632	1603.607	420.251	1725.795	-32.194
2900	751.092	1750.670	1171.837	1678.615	420.376	1772.409	-31.924
3000	752.955	1776.165	1191.558	1753.819	420.318	1819.041	-31.672
3100	754.656	1800.882	1210.817	1829.201	420.020	1865.623	-31.435
3200	756.213	1824.867	1229.634	1904.745	419.512	1912.272	-31.214
3300	757.640	1848.159	1248.026	1980.439	418.782	1958.969	-31.007
3400	758.953	1870.796	1266.011	2056.270	417.808	2005.628	-30.812
3500	760.162	1892.814	1283.607	2132.226	416.595	2052.306	-30.628
3600	761.278	1914.244	1300.828	2208.299	415.158	2099.086	-30.456
3700	762.310	1935.117	1317.690	2284.479	413.474	2145.922	-30.294
3800	763.267	1955.459	1334.207	2360.759	411.523	2192.761	-30.141
3900	764.155	1975.297	1350.392	2437.130	409.337	2239.619	-29.996
4000	764.981	1994.654	1366.257	2513.587	406.902	2286.637	-29.860
4100	765.750	2013.553	1381.816	2590.124	404.193	2333.665	-29.731
4200	766.467	2032.015	1397.078	2666.736	401.230	2380.755	-29.608
4300	767.137	2050.058	1412.054	2743.416	398.003	2427.853	-29.492
4400	767.764	2067.701	1426.755	2820.162	394.518	2475.097	-29.383
4500	768.351	2084.962	1441.191	2896.968	390.786	2522.465	-29.279
4600	768.902	2101.855	1455.370	2973.831	386.769	2569.923	-29.182
4700	769.420	2118.397	1469.302	3050.747	382.478	2617.388	-29.088
4800	769.907	2134.601	1482.994	3127.714	377.946	2665.025	-29.001
4900	770.365	2150.481	1496.455	3204.727	373.120	2712.660	-28.917
5000	770.797	2166.049	1509.692	3281.786	368.069	2760.535	-28.839

3.61. Indeno[2,1-*a*]phenalene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 200-71-5
Point Group: C_s

Length: 13.41 Å
Width: 9.192 Å
Breadth: 3.885 Å
L/B Ratio: 1.459

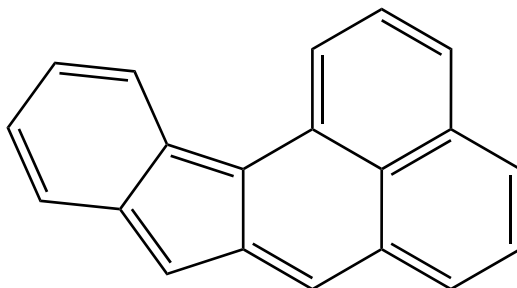
Cartesian coordinates:

C	-4.1033	-1.1794	0.0000	C	1.8419	0.0264	0.0000	H	-5.4579	1.9555	0.0000
C	-2.7679	-0.8200	0.0000	C	0.9457	-1.0907	0.0000	H	-6.1233	-0.4239	0.0000
C	-2.3870	0.5513	0.0000	C	1.4470	-2.3740	0.0000	H	-4.4025	-2.2317	0.0000
C	-3.3387	1.5522	0.0000	C	2.8405	-2.5988	0.0000	H	-0.4170	2.6708	0.0000
C	-4.6865	1.1784	0.0000	C	3.7159	-1.5466	0.0000	H	5.2074	0.6949	0.0000
C	-5.0604	-0.1602	0.0000	C	3.2322	-0.2097	0.0000	H	4.3407	3.0241	0.0000
C	-0.9231	0.5966	0.0000	C	2.2626	2.4210	0.0000	H	1.9031	3.4565	0.0000
C	-0.4731	-0.8121	0.0000	C	3.6497	2.1746	0.0000	H	0.7655	-3.2326	0.0000
C	-1.5548	-1.6416	0.0000	C	4.1289	0.8902	0.0000	H	3.2110	-3.6293	0.0000
C	-0.0678	1.6317	0.0000	H	-1.5637	-2.7304	0.0000	H	4.7985	-1.7172	0.0000
C	1.3638	1.3736	0.0000	H	-3.0461	2.6068	0.0000				

Table 3.61: Table of thermodynamic data as a function of temperature for Indeno[2,1-*a*]phenalene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-37.855	387.265	387.265	∞
100	83.251	314.444	638.933	-32.449	407.444	438.340	-228.961
200	162.041	394.890	496.859	-20.394	396.815	473.460	-123.653
250	208.522	435.998	480.555	-11.139	391.774	493.204	-103.047
298.15	254.088	476.629	476.629	0.000	387.265	513.160	-89.902
300	255.820	478.206	476.634	0.472	387.099	513.940	-89.483
350	301.393	521.097	479.917	14.413	382.926	535.419	-79.905
400	343.670	564.145	487.756	30.556	379.287	557.451	-72.794
450	381.960	606.874	498.622	48.713	376.119	579.915	-67.313
500	416.177	648.924	511.557	68.684	373.357	602.726	-62.965
600	473.554	730.081	541.275	113.284	368.823	649.048	-56.503
700	518.961	806.622	573.771	162.996	365.447	696.039	-51.938
800	555.427	878.386	607.412	216.779	363.092	743.430	-48.540
900	585.193	945.581	641.294	273.859	361.628	791.058	-45.911
1000	609.822	1008.552	674.905	333.647	360.932	838.816	-43.814
1100	630.419	1067.669	707.951	395.689	360.860	886.620	-42.101
1200	647.788	1123.288	740.268	459.623	361.307	934.393	-40.672
1300	662.540	1175.737	771.768	525.159	362.137	982.121	-39.461
1400	675.146	1225.310	802.410	592.060	363.253	1029.777	-38.421
1500	685.977	1272.269	832.182	660.130	364.595	1077.346	-37.516
1600	695.334	1316.846	861.093	729.206	366.066	1124.814	-36.721
1700	703.458	1359.250	889.159	799.155	367.611	1172.169	-36.016
1800	710.543	1399.664	916.407	869.863	369.175	1219.480	-35.388
1900	716.752	1438.251	942.864	941.235	370.734	1266.666	-34.822
2000	722.216	1475.157	968.563	1013.189	372.248	1313.789	-34.312
2100	727.045	1510.514	993.534	1085.657	373.660	1360.829	-33.848
2200	731.330	1544.437	1017.810	1158.580	374.969	1407.806	-33.425
2300	735.146	1577.031	1041.420	1231.907	376.170	1454.725	-33.037
2400	738.557	1608.392	1064.394	1305.596	377.213	1501.559	-32.680
2500	741.617	1638.605	1086.762	1379.607	378.104	1548.437	-32.352
2600	744.371	1667.746	1108.551	1453.909	378.818	1595.196	-32.047
2700	746.857	1695.886	1129.786	1528.472	379.358	1641.984	-31.765
2800	749.108	1723.089	1150.492	1603.272	379.704	1688.773	-31.504
2900	751.151	1749.413	1170.693	1678.287	379.834	1735.513	-31.259
3000	753.012	1774.910	1190.411	1753.496	379.782	1782.271	-31.031
3100	754.711	1799.629	1209.666	1828.884	379.489	1828.978	-30.817
3200	756.265	1823.615	1228.479	1904.434	378.987	1875.752	-30.618
3300	757.690	1846.908	1246.868	1980.133	378.262	1922.574	-30.431
3400	759.001	1869.548	1264.851	2055.968	377.293	1969.358	-30.255
3500	760.208	1891.567	1282.444	2131.929	376.085	2016.161	-30.089
3600	761.322	1912.998	1299.663	2208.006	374.652	2063.065	-29.934
3700	762.353	1933.872	1316.523	2284.191	372.972	2110.026	-29.788
3800	763.308	1954.215	1333.038	2360.475	371.026	2156.990	-29.649
3900	764.194	1974.054	1349.221	2436.850	368.843	2203.972	-29.518
4000	765.018	1993.413	1365.085	2513.311	366.413	2251.114	-29.396
4100	765.786	2012.312	1380.641	2589.852	363.707	2298.266	-29.280
4200	766.502	2030.775	1395.902	2666.467	360.748	2345.480	-29.170
4300	767.171	2048.819	1410.877	2743.151	357.524	2392.702	-29.065
4400	767.796	2066.463	1425.577	2819.899	354.043	2440.070	-28.967
4500	768.382	2083.724	1440.011	2896.709	350.314	2487.562	-28.874
4600	768.932	2100.618	1454.189	2973.575	346.300	2535.144	-28.787
4700	769.449	2117.161	1468.120	3050.494	342.011	2582.733	-28.703
4800	769.934	2133.365	1481.811	3127.463	337.483	2630.493	-28.625
4900	770.392	2149.246	1495.270	3204.480	332.659	2678.252	-28.550
5000	770.823	2164.814	1508.506	3281.541	327.610	2726.250	-28.480

3.62. Indeno[1,2-*a*]phenalene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 198-19-6
Point Group: C_s

Length: 13.64 Å
Width: 9.637 Å
Breadth: 3.884 Å
L/B Ratio: 1.415

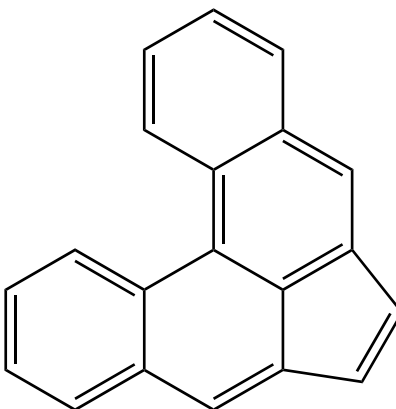
Cartesian coordinates:

C	2.7511	1.5138	0.0000	C	-0.5024	0.7296	0.0000	H	-3.0804	-3.1387	0.0000
C	2.0456	0.2670	0.0000	C	0.7057	-0.0545	0.0000	H	0.4537	2.6576	0.0000
C	2.8213	-0.9842	0.0000	C	-3.0321	-2.0433	0.0000	H	-1.6749	3.9278	0.0000
C	4.2552	-0.9216	0.0000	C	-4.2285	-1.3022	0.0000	H	-3.8574	2.7383	0.0000
C	4.8631	0.2873	0.0000	C	-4.1966	0.0692	0.0000	H	-0.6390	-3.2654	0.0000
C	4.1052	1.5135	0.0000	C	-2.9570	0.7591	0.0000	H	2.2190	-3.1128	0.0000
C	1.9679	-2.0549	0.0000	C	-0.5010	2.1102	0.0000	H	4.8212	-1.8583	0.0000
C	0.6055	-1.5263	0.0000	C	-1.7114	2.8332	0.0000	H	5.9553	0.3647	0.0000
C	-0.5775	-2.1707	0.0000	C	-2.9145	2.1797	0.0000	H	4.6631	2.4557	0.0000
C	-1.8082	-1.4014	0.0000	H	-5.1266	0.6495	0.0000	H	2.1688	2.4457	0.0000
C	-1.7517	0.0262	0.0000	H	-5.1856	-1.8345	0.0000				

Table 3.62: Table of thermodynamic data as a function of temperature for Indeno[1,2-*a*]phenalene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-38.109	459.505	459.505	∞
100	83.238	315.536	642.284	-32.675	479.459	510.245	-266.519
200	163.344	396.332	499.138	-20.561	468.888	545.244	-142.400
250	210.277	437.786	482.702	-11.229	463.924	564.908	-118.029
298.15	256.016	478.744	478.744	0.000	459.505	584.769	-102.447
300	257.751	480.333	478.749	0.475	459.343	585.545	-101.950
350	303.337	523.525	482.056	14.514	455.268	606.910	-90.575
400	345.545	566.828	489.947	30.752	451.724	628.815	-82.113
450	383.728	609.772	500.880	49.001	448.647	651.139	-75.581
500	417.821	652.002	513.888	69.057	445.970	673.800	-70.390
600	474.939	733.436	543.755	113.809	441.588	719.800	-62.663
700	520.103	810.172	576.391	163.646	438.338	766.445	-57.192
800	556.359	882.074	610.157	217.533	436.087	813.474	-53.113
900	585.949	949.368	644.150	274.697	434.706	860.728	-49.954
1000	610.436	1012.411	677.858	334.553	434.079	908.104	-47.433
1100	630.919	1071.581	710.989	396.651	434.062	955.519	-45.373
1200	648.199	1127.240	743.381	460.631	434.554	1002.899	-43.654
1300	662.879	1179.718	774.946	526.204	435.421	1050.230	-42.198
1400	675.427	1229.314	805.646	593.136	436.569	1097.486	-40.947
1500	686.214	1276.291	835.470	661.231	437.936	1144.654	-39.860
1600	695.534	1320.883	864.427	730.329	439.429	1191.719	-38.905
1700	703.628	1363.298	892.535	800.297	440.992	1238.670	-38.059
1800	710.689	1403.720	919.820	871.021	442.572	1285.576	-37.306
1900	716.878	1442.315	946.312	942.406	444.145	1332.355	-36.628
2000	722.326	1479.227	972.042	1014.372	445.671	1379.072	-36.017
2100	727.141	1514.589	997.041	1086.850	447.093	1425.704	-35.462
2200	731.415	1548.516	1021.342	1159.782	448.411	1472.274	-34.956
2300	735.221	1581.114	1044.976	1233.117	449.621	1518.784	-34.492
2400	738.624	1612.478	1067.973	1306.813	450.670	1565.211	-34.065
2500	741.677	1642.693	1090.361	1380.830	451.568	1611.680	-33.674
2600	744.425	1671.837	1112.168	1455.138	452.287	1658.030	-33.310
2700	746.906	1699.979	1133.421	1529.706	452.832	1704.409	-32.973
2800	749.152	1727.183	1154.144	1604.511	453.183	1750.788	-32.661
2900	751.192	1753.508	1174.360	1679.530	453.317	1797.119	-32.369
3000	753.049	1779.007	1194.092	1754.743	453.269	1843.467	-32.097
3100	754.745	1803.727	1213.361	1830.134	452.980	1889.765	-31.842
3200	756.296	1827.714	1232.187	1905.688	452.481	1936.129	-31.603
3300	757.719	1851.009	1250.588	1981.389	451.759	1982.541	-31.380
3400	759.028	1873.648	1268.582	2057.228	450.793	2028.915	-31.170
3500	760.233	1895.668	1286.185	2133.191	449.587	2075.307	-30.972
3600	761.345	1917.101	1303.414	2209.271	448.156	2121.801	-30.786
3700	762.374	1937.975	1320.284	2285.458	446.479	2168.352	-30.611
3800	763.328	1958.319	1336.808	2361.743	444.535	2214.906	-30.445
3900	764.213	1978.158	1352.999	2438.121	442.354	2261.477	-30.288
4000	765.036	1997.517	1368.871	2514.584	439.925	2308.209	-30.141
4100	765.802	2016.417	1384.435	2591.126	437.222	2354.950	-30.002
4200	766.517	2034.880	1399.703	2667.743	434.264	2401.754	-29.870
4300	767.185	2052.924	1414.685	2744.428	431.042	2448.565	-29.744
4400	767.810	2070.569	1429.392	2821.178	427.562	2495.523	-29.625
4500	768.396	2087.830	1443.833	2897.989	423.834	2542.604	-29.513
4600	768.945	2104.725	1458.017	2974.856	419.822	2589.775	-29.407
4700	769.461	2121.268	1471.953	3051.777	415.534	2636.953	-29.306
4800	769.946	2137.473	1485.650	3128.747	411.007	2684.303	-29.211
4900	770.403	2153.353	1499.115	3205.765	406.185	2731.651	-29.119
5000	770.833	2168.922	1512.356	3282.827	401.137	2779.238	-29.034

3.63. Benz[*a*]acephenanthrylene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 192-28-9
Point Group: C₂

Length: 12.23 Å
Width: 10.49 Å
Breadth: 4.366 Å
L/B Ratio: 1.166

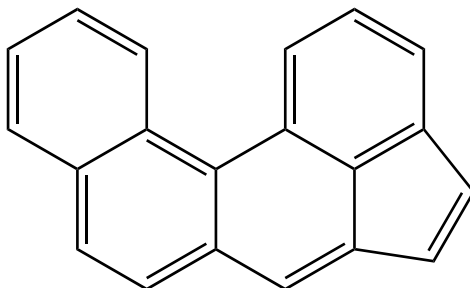
Cartesian coordinates:

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C	-1.1635	2.1235	-0.0881	C	2.3864	1.5493	0.1846	H	-2.9260	-3.7035	0.4562
C	-2.3864	1.5494	-0.1844	C	1.3173	-0.7066	-0.0377	H	-4.9137	-2.2763	0.0179
C	-2.4669	0.1145	-0.1072	C	2.4670	0.1145	0.1074	H	-4.6285	0.1719	-0.2817
C	-1.3172	-0.7066	0.0374	C	3.7542	-0.4729	0.1317	H	3.3030	2.1390	0.2925
C	-1.5307	-2.0838	0.2759	C	3.9165	-1.8253	-0.0409	H	4.6284	0.1717	0.2827
C	-2.7913	-2.6324	0.2725	C	2.7913	-2.6323	-0.2727	H	4.9136	-2.2764	-0.0168
C	-3.9166	-1.8252	0.0415	C	1.5308	-2.0837	-0.2765	H	2.9260	-3.7035	-0.4565
C	-3.7543	-0.4728	-0.1311	H	-1.3362	4.3757	-0.1127	H	0.6782	-2.7377	-0.4996
C	-0.0000	-0.0967	-0.0002	H	1.3363	4.3757	0.1126				

Table 3.63: Table of thermodynamic data as a function of temperature for Benz[*a*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-37.520	404.298	404.298	∞
100	81.817	305.661	627.989	-32.233	424.693	456.468	-238.429
200	160.980	385.263	486.749	-20.297	413.945	492.515	-128.629
250	207.536	426.142	470.518	-11.094	408.852	512.747	-107.130
298.15	253.194	466.607	466.607	0.000	404.298	533.180	-93.409
300	254.930	468.178	466.612	0.470	404.130	533.979	-92.972
350	300.605	510.941	469.885	14.370	399.916	555.963	-82.971
400	342.976	553.889	477.702	30.475	396.239	578.506	-75.544
450	381.345	596.541	488.541	48.600	393.038	601.485	-69.817
500	415.622	638.529	501.447	68.541	390.247	624.814	-65.272
600	473.071	719.593	531.109	113.090	385.662	672.180	-58.517
700	518.506	796.062	563.555	162.755	382.239	720.223	-53.743
800	554.978	867.765	597.148	216.494	379.840	768.674	-50.188
900	584.744	934.908	630.988	273.528	378.330	817.367	-47.438
1000	609.374	997.831	664.560	333.272	377.590	866.195	-45.244
1100	629.976	1056.905	697.570	395.269	377.473	915.072	-43.452
1200	647.356	1112.487	729.854	459.160	377.876	963.924	-41.958
1300	662.122	1164.902	761.322	524.653	378.663	1012.734	-40.691
1400	674.745	1214.444	791.935	591.513	379.739	1061.474	-39.603
1500	685.596	1261.376	821.680	659.543	381.041	1110.132	-38.657
1600	694.973	1305.930	850.566	728.583	382.475	1158.690	-37.827
1700	703.116	1348.312	878.608	798.497	383.985	1207.138	-37.090
1800	710.221	1388.707	905.834	869.171	385.516	1255.544	-36.434
1900	716.448	1427.277	932.271	940.512	387.044	1303.826	-35.844
2000	721.931	1464.168	957.950	1012.436	388.529	1352.048	-35.311
2100	726.777	1499.511	982.903	1084.877	389.913	1400.187	-34.827
2200	731.077	1533.422	1007.161	1157.774	391.196	1448.265	-34.385
2300	734.908	1566.006	1030.755	1231.076	392.373	1496.285	-33.981
2400	738.333	1597.357	1053.715	1304.742	393.392	1544.223	-33.608
2500	741.406	1627.561	1076.068	1378.731	394.262	1592.205	-33.267
2600	744.172	1656.694	1097.843	1453.013	394.955	1640.069	-32.949
2700	746.669	1684.827	1119.065	1527.557	395.475	1687.963	-32.655
2800	748.930	1712.023	1139.759	1602.339	395.803	1735.858	-32.382
2900	750.983	1738.340	1159.949	1677.336	395.916	1783.704	-32.127
3000	752.853	1763.832	1179.655	1752.529	395.847	1831.570	-31.890
3100	754.560	1788.546	1198.901	1827.901	395.539	1879.385	-31.667
3200	756.122	1812.527	1217.704	1903.436	395.023	1927.268	-31.459
3300	757.555	1835.817	1236.083	1979.121	394.283	1975.199	-31.264
3400	758.872	1858.452	1254.057	2054.943	393.302	2023.092	-31.080
3500	760.085	1880.467	1271.641	2130.892	392.080	2071.004	-30.907
3600	761.205	1901.896	1288.852	2206.957	390.636	2119.019	-30.746
3700	762.241	1922.766	1305.704	2283.130	388.945	2167.090	-30.593
3800	763.201	1943.107	1322.211	2359.403	386.987	2215.165	-30.449
3900	764.092	1962.943	1338.387	2435.768	384.794	2263.257	-30.312
4000	764.921	1982.299	1354.244	2512.219	382.354	2311.511	-30.185
4100	765.693	2001.196	1369.793	2588.751	379.639	2359.775	-30.063
4200	766.413	2019.656	1385.047	2665.356	376.670	2408.101	-29.948
4300	767.085	2037.698	1400.016	2742.032	373.438	2456.434	-29.839
4400	767.714	2055.340	1414.710	2818.772	369.948	2504.914	-29.737
4500	768.304	2072.600	1429.139	2895.573	366.211	2553.518	-29.640
4600	768.857	2089.492	1443.312	2972.431	362.190	2602.213	-29.548
4700	769.376	2106.033	1457.237	3049.343	357.894	2650.915	-29.461
4800	769.865	2122.236	1470.923	3126.306	353.358	2699.788	-29.379
4900	770.325	2138.115	1484.377	3203.315	348.528	2748.659	-29.300
5000	770.758	2153.682	1497.608	3280.370	343.472	2797.771	-29.228

3.64. Benz[*l*]acephenanthrylene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 95690-49-6
Point Group: C₁

Length: 12.96 Å
Width: 9.324 Å
Breadth: 4.509 Å
L/B Ratio: 1.390

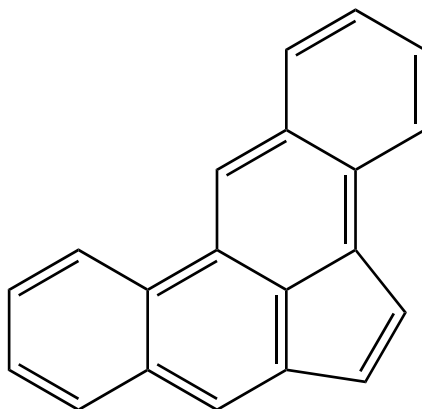
Cartesian coordinates:

C	3.6637	-1.5974	-0.2440	C	-0.4013	-0.2414	0.0156	H	4.2239	2.5876	0.1741
C	4.2754	-0.3844	-0.1710	C	-2.5496	-2.0865	0.2720	H	2.0615	3.7697	0.5005
C	3.2558	0.6671	-0.0222	C	-1.2756	-2.5395	0.1705	H	-0.0794	2.6080	0.4835
C	3.2856	2.0257	0.1522	C	-2.8247	-0.6923	0.1324	H	1.2217	-3.3183	-0.1122
C	2.0474	2.6877	0.3275	C	-1.7682	0.2252	-0.0541	H	-3.3859	-2.7773	0.4299
C	0.8359	2.0299	0.3014	C	-2.1229	1.5623	-0.3625	H	-1.0620	-3.6141	0.2196
C	2.2069	-1.4103	-0.1504	C	-3.4326	1.9740	-0.3826	H	-1.3411	2.2881	-0.6210
C	1.9935	0.0059	-0.0440	C	-4.4705	1.0666	-0.1039	H	-3.6797	3.0134	-0.6228
C	0.7577	0.6282	0.0754	C	-4.1698	-0.2501	0.1356	H	-5.5085	1.4142	-0.0985
C	1.1277	-2.2270	-0.0838	H	4.1362	-2.5716	-0.3510	H	-4.9674	-0.9787	0.3219
C	-0.1792	-1.6319	0.0262	H	5.3434	-0.1795	-0.2091				

Table 3.64: Table of thermodynamic data as a function of temperature for Benz[*l*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-37.614	413.273	413.273	∞
100	81.972	312.819	635.575	-32.276	433.625	464.684	-242.721
200	161.124	392.424	494.122	-20.340	422.877	500.015	-130.588
250	207.988	433.369	477.855	-11.122	417.799	519.887	-108.622
298.15	253.867	473.933	473.933	0.000	413.273	539.971	-94.599
300	255.610	475.509	473.938	0.471	413.106	540.756	-94.152
350	301.421	518.387	477.220	14.409	408.930	562.370	-83.927
400	343.861	561.450	485.058	30.557	405.296	584.538	-76.331
450	382.251	604.208	495.926	48.727	402.140	607.136	-70.473
500	416.519	646.291	508.866	68.713	399.394	630.079	-65.823
600	473.903	727.513	538.599	113.349	394.896	676.661	-58.907
700	519.249	804.104	571.115	163.093	391.552	723.906	-54.017
800	555.633	875.901	604.775	216.901	389.222	771.548	-50.376
900	585.319	943.116	638.675	273.997	387.774	819.423	-47.557
1000	609.880	1006.096	672.302	333.794	387.087	867.427	-45.309
1100	630.423	1065.216	705.362	395.839	387.018	915.476	-43.471
1200	647.752	1120.833	737.690	459.772	387.463	963.495	-41.939
1300	662.475	1173.278	769.199	525.303	388.288	1011.468	-40.640
1400	675.061	1222.846	799.849	592.196	389.397	1059.370	-39.525
1500	685.880	1269.798	829.627	660.256	390.729	1107.186	-38.555
1600	695.229	1314.369	858.543	729.323	392.190	1154.901	-37.703
1700	703.347	1356.767	886.613	799.261	393.724	1202.505	-36.948
1800	710.432	1397.174	913.864	869.958	395.277	1250.064	-36.275
1900	716.641	1435.755	940.324	941.318	396.825	1297.499	-35.670
2000	722.107	1472.656	966.025	1013.261	398.328	1344.873	-35.124
2100	726.938	1508.007	990.998	1085.718	399.729	1392.163	-34.627
2200	731.226	1541.925	1015.275	1158.631	401.028	1439.391	-34.175
2300	735.046	1574.515	1038.885	1231.948	402.219	1486.561	-33.760
2400	738.461	1605.872	1061.861	1305.627	403.252	1533.647	-33.378
2500	741.525	1636.081	1084.229	1379.629	404.134	1580.777	-33.028
2600	744.282	1665.218	1106.018	1453.921	404.838	1627.789	-32.702
2700	746.772	1693.355	1127.253	1528.476	405.369	1674.830	-32.401
2800	749.026	1720.555	1147.959	1603.268	405.707	1721.872	-32.121
2900	751.074	1746.876	1168.160	1678.274	405.829	1768.865	-31.860
3000	752.938	1772.370	1187.878	1753.476	405.769	1815.877	-31.617
3100	754.640	1797.087	1207.133	1828.857	405.470	1862.839	-31.388
3200	756.197	1821.071	1225.946	1904.400	404.961	1909.867	-31.175
3300	757.626	1844.362	1244.335	1980.092	404.229	1956.944	-30.975
3400	758.939	1866.999	1262.317	2055.921	403.254	2003.983	-30.787
3500	760.149	1889.017	1279.909	2131.876	402.039	2051.040	-30.609
3600	761.265	1910.447	1297.128	2207.948	400.601	2098.199	-30.443
3700	762.298	1931.319	1313.988	2284.126	398.915	2145.415	-30.287
3800	763.256	1951.661	1330.502	2360.405	396.964	2192.635	-30.139
3900	764.144	1971.499	1346.684	2436.775	394.776	2239.872	-29.999
4000	764.970	1990.856	1362.548	2513.231	392.340	2287.270	-29.868
4100	765.740	2009.754	1378.104	2589.767	389.630	2334.677	-29.744
4200	766.457	2028.215	1393.364	2666.378	386.667	2382.148	-29.626
4300	767.128	2046.258	1408.338	2743.057	383.438	2429.626	-29.513
4400	767.755	2063.902	1423.038	2819.802	379.953	2477.249	-29.408
4500	768.343	2081.162	1437.472	2896.607	376.220	2524.997	-29.309
4600	768.894	2098.055	1451.649	2973.469	372.202	2572.836	-29.215
4700	769.412	2114.597	1465.579	3050.385	367.910	2620.681	-29.125
4800	769.899	2130.801	1479.270	3127.351	363.378	2668.698	-29.041
4900	770.358	2146.680	1492.729	3204.364	358.551	2716.713	-28.960
5000	770.790	2162.248	1505.964	3281.421	353.498	2764.967	-28.885

3.65. Benz[*e*]aceanthrylene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 199-54-2
Point Group: C_s

Length: 13.85 Å
Width: 9.514 Å
Breadth: 4.172 Å
L/B Ratio: 1.456

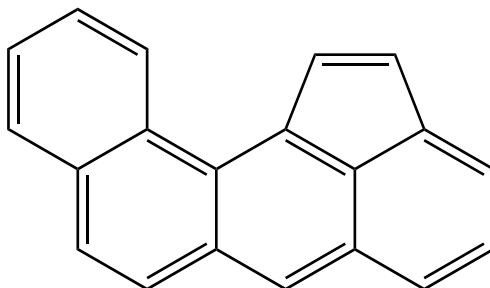
Cartesian coordinates:

C	1.3946	2.7282	-0.0116	C	4.6659	-0.3565	-0.0012	H	0.2975	-2.5062	0.0059
C	-0.0238	3.2084	-0.0090	C	4.2786	-1.7217	0.0036	H	-2.9593	2.5975	-0.0010
C	1.3303	1.2826	-0.0073	C	2.9591	-2.0707	0.0041	H	3.9931	1.6962	-0.0094
C	0.5783	-1.4424	0.0029	C	-2.7307	0.4094	0.0031	H	5.7327	-0.1088	-0.0013
C	-0.9040	1.9885	-0.0047	C	-1.8560	-0.7007	0.0040	H	5.0572	-2.4918	0.0065
C	-0.0057	0.8609	-0.0037	C	-2.3835	-2.0024	0.0058	H	2.6587	-3.1248	0.0063
C	-0.4218	-0.4773	0.0017	C	-3.7495	-2.2033	0.0075	H	-1.6862	-2.8517	0.0049
C	-2.2357	1.7749	-0.0007	C	-4.6198	-1.1069	0.0076	H	-4.1565	-3.2197	0.0089
C	1.9421	-1.0686	0.0008	C	-4.1192	0.1802	0.0054	H	-5.7018	-1.2753	0.0100
C	2.3404	0.2992	-0.0043	H	-0.1842	3.8512	0.8772	H	-4.8042	1.0362	0.0058
C	3.7235	0.6320	-0.0056	H	-0.1891	3.8493	-0.8957				

Table 3.65: Table of thermodynamic data as a function of temperature for Benz[e]aceanthrylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-38.922	392.476	392.476	∞
100	87.845	316.800	650.145	-33.335	411.770	442.430	-231.097
200	166.678	400.711	504.609	-20.780	401.641	477.121	-124.609
250	212.412	442.772	488.021	-11.312	396.812	496.549	-103.746
298.15	257.416	484.037	484.037	0.000	392.476	516.162	-90.428
300	259.131	485.634	484.042	0.478	392.316	516.928	-90.003
350	304.321	529.005	487.364	14.575	388.299	538.023	-80.294
400	346.348	572.426	495.285	30.857	384.799	559.651	-73.081
450	384.465	615.461	506.252	49.144	381.760	581.693	-67.520
500	418.551	657.767	519.296	69.236	379.120	604.067	-63.105
600	475.729	739.339	549.233	114.063	374.813	649.483	-56.541
700	520.979	816.203	581.940	163.984	371.647	695.532	-51.900
800	557.310	888.227	615.774	217.963	369.487	741.952	-48.443
900	586.950	955.637	649.832	275.224	368.204	788.584	-45.767
1000	611.459	1018.787	683.604	335.182	367.678	835.328	-43.632
1100	631.940	1078.054	716.797	397.382	367.764	882.100	-41.887
1200	649.200	1133.801	749.248	461.463	368.357	928.828	-40.430
1300	663.847	1186.359	780.870	527.135	369.323	975.500	-39.195
1400	676.355	1236.025	811.624	594.161	370.566	1022.088	-38.134
1500	687.096	1283.064	841.499	662.347	372.023	1068.582	-37.211
1600	696.369	1327.711	870.504	731.532	373.602	1114.966	-36.399
1700	704.415	1370.175	898.658	801.580	375.246	1161.232	-35.680
1800	711.430	1410.642	925.986	872.380	376.902	1207.448	-35.039
1900	717.574	1449.275	952.519	943.837	378.547	1253.534	-34.461
2000	722.980	1486.222	978.287	1015.871	380.141	1299.553	-33.940
2100	727.756	1521.614	1003.323	1088.412	381.626	1345.484	-33.466
2200	731.992	1555.569	1027.658	1161.404	383.004	1391.349	-33.034
2300	735.764	1588.192	1051.325	1234.795	384.269	1437.153	-32.638
2400	739.135	1619.579	1074.352	1308.543	385.371	1482.870	-32.273
2500	742.157	1649.814	1096.770	1382.610	386.319	1528.629	-31.938
2600	744.877	1678.976	1118.605	1456.965	387.085	1574.266	-31.627
2700	747.332	1707.135	1139.884	1531.577	387.673	1619.930	-31.339
2800	749.555	1734.354	1160.632	1606.423	388.065	1665.593	-31.071
2900	751.572	1760.693	1180.872	1681.481	388.239	1711.206	-30.822
3000	753.409	1786.204	1200.626	1756.732	388.228	1756.835	-30.589
3100	755.086	1810.936	1219.917	1832.158	387.974	1802.412	-30.370
3200	756.620	1834.933	1238.763	1907.744	387.508	1848.055	-30.166
3300	758.026	1858.237	1257.184	1983.477	386.818	1893.745	-29.975
3400	759.319	1880.886	1275.196	2059.346	385.882	1939.395	-29.795
3500	760.510	1902.914	1292.818	2135.338	384.704	1985.064	-29.625
3600	761.610	1924.354	1310.064	2211.445	383.301	2030.833	-29.466
3700	762.626	1945.236	1326.950	2287.657	381.649	2076.658	-29.317
3800	763.568	1965.586	1343.490	2363.967	379.729	2122.485	-29.175
3900	764.442	1985.432	1359.696	2440.368	377.573	2168.329	-29.041
4000	765.255	2004.796	1375.583	2516.854	375.166	2214.334	-28.916
4100	766.012	2023.702	1391.161	2593.418	372.484	2260.347	-28.797
4200	766.718	2042.169	1406.442	2670.054	369.547	2306.422	-28.684
4300	767.378	2060.218	1421.437	2746.760	366.344	2352.504	-28.577
4400	767.995	2077.867	1436.156	2823.529	362.883	2398.732	-28.476
4500	768.573	2095.133	1450.609	2900.357	359.173	2445.082	-28.381
4600	769.115	2112.031	1464.805	2977.242	355.178	2491.524	-28.292
4700	769.624	2128.577	1478.752	3054.179	350.907	2537.971	-28.206
4800	770.103	2144.786	1492.459	3131.166	346.396	2584.590	-28.125
4900	770.554	2160.669	1505.935	3208.199	341.589	2631.206	-28.048
5000	770.979	2176.241	1519.186	3285.276	336.556	2678.062	-27.977

3.66. Benz[*l*]aceanthrylene



Other names: Naphth[1,2-*d*]acenaphthylene

Formula: C₂₀H₁₂

Mass: 252.309 g/mol

CAS Number: 211-91-6

Point Group: C_s

Length: 13.54 Å

Width: 9.169 Å

Breadth: 3.927 Å

L/B Ratio: 1.477

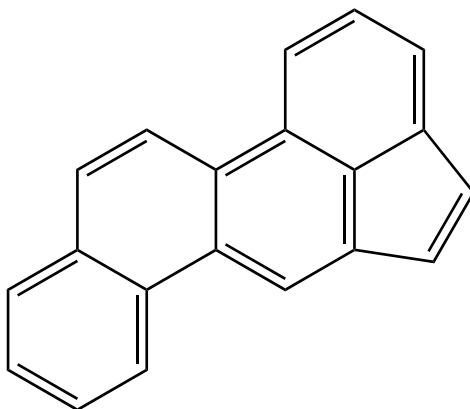
Cartesian coordinates:

C	4.2443	0.4020	0.0125	C	-1.9155	-0.2086	0.0006	H	-3.9285	2.5193	-0.0242
C	2.8804	0.7489	0.0103	C	-2.2385	1.1435	-0.0094	H	-5.6327	0.7237	-0.0161
C	1.8851	-0.2488	-0.0046	C	-1.1467	2.0294	-0.0086	H	-5.0088	-1.6764	0.0053
C	2.3127	-1.5901	-0.0275	C	-3.6303	1.4655	-0.0157	H	-1.3313	3.1106	-0.0118
C	3.6527	-1.9219	-0.0265	C	-4.5678	0.4662	-0.0110	H	3.3222	2.8875	0.0299
C	4.6296	-0.9218	-0.0042	C	-4.2196	-0.9184	0.0011	H	0.9476	3.5757	0.0097
C	0.4775	0.1336	0.0000	C	-2.8977	-1.2533	0.0072	H	1.5788	-2.4040	-0.0494
C	0.1576	1.5386	-0.0018	C	-2.1317	-2.5051	0.0217	H	3.9557	-2.9741	-0.0436
C	1.2240	2.5142	0.0083	C	-0.8023	-2.2121	0.0225	H	5.6903	-1.1925	-0.0018
C	2.5178	2.1428	0.0184	H	0.0036	-2.9465	0.0359	H	4.9995	1.1964	0.0269
C	-0.6003	-0.7480	0.0069	H	-2.5891	-3.4922	0.0314				

Table 3.66: Table of thermodynamic data as a function of temperature for Benz[*l*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-37.639	417.371	417.371	∞
100	81.952	314.688	637.192	-32.250	437.749	468.620	-244.777
200	161.011	394.244	495.854	-20.322	426.993	503.767	-131.568
250	207.812	435.157	479.601	-11.111	421.908	523.549	-109.387
298.15	253.601	475.684	475.684	0.000	417.371	543.547	-95.225
300	255.340	477.258	475.689	0.471	417.204	544.329	-94.774
350	301.060	520.087	478.967	14.392	413.011	565.857	-84.448
400	343.429	563.097	486.796	30.520	409.357	587.941	-76.776
450	381.774	605.801	497.651	48.668	406.179	610.458	-70.859
500	416.021	647.833	510.574	68.629	403.408	633.323	-66.161
600	473.409	728.964	540.272	113.215	398.860	679.755	-59.177
700	518.793	805.481	572.750	162.911	395.468	726.859	-54.238
800	555.224	877.220	606.374	216.676	393.095	774.366	-50.560
900	584.957	944.389	640.241	273.734	391.609	822.112	-47.713
1000	609.560	1007.334	673.836	333.497	390.888	869.991	-45.443
1100	630.141	1066.424	706.868	395.512	390.789	917.917	-43.587
1200	647.503	1122.019	739.171	459.418	391.207	965.816	-42.040
1300	662.253	1174.445	770.656	524.926	392.009	1013.672	-40.729
1400	674.863	1223.997	801.284	591.798	393.097	1061.458	-39.603
1500	685.702	1270.936	831.044	659.839	394.410	1109.160	-38.624
1600	695.069	1315.497	859.941	728.889	395.854	1156.761	-37.764
1700	703.203	1357.885	887.996	798.812	397.373	1204.253	-37.001
1800	710.300	1398.284	915.232	869.495	398.912	1251.701	-36.323
1900	716.521	1436.859	941.678	940.843	400.448	1299.025	-35.712
2000	721.997	1473.753	967.366	1012.774	401.939	1346.288	-35.161
2100	726.838	1509.099	992.327	1085.221	403.330	1393.469	-34.660
2200	731.134	1543.013	1016.593	1158.124	404.619	1440.588	-34.203
2300	734.961	1575.599	1040.194	1231.432	405.801	1487.649	-33.785
2400	738.382	1606.952	1063.160	1305.103	406.826	1534.628	-33.400
2500	741.452	1637.158	1085.519	1379.097	407.700	1581.650	-33.046
2600	744.214	1666.293	1107.300	1453.383	408.398	1628.554	-32.717
2700	746.708	1694.428	1128.527	1527.931	408.922	1675.488	-32.414
2800	748.967	1721.625	1149.226	1602.716	409.253	1722.423	-32.132
2900	751.018	1747.944	1169.420	1677.717	409.370	1769.309	-31.868
3000	752.886	1773.436	1189.132	1752.914	409.305	1816.214	-31.622
3100	754.591	1798.151	1208.381	1828.289	409.000	1863.069	-31.392
3200	756.151	1822.134	1227.188	1903.827	408.486	1909.991	-31.177
3300	757.582	1845.424	1245.571	1979.515	407.750	1956.961	-30.975
3400	758.898	1868.060	1263.548	2055.340	406.771	2003.894	-30.785
3500	760.110	1890.076	1281.136	2131.291	405.552	2050.846	-30.607
3600	761.229	1911.505	1298.350	2207.359	404.110	2097.899	-30.439
3700	762.263	1932.376	1315.205	2283.534	402.421	2145.009	-30.281
3800	763.222	1952.717	1331.715	2359.809	400.466	2192.123	-30.132
3900	764.112	1972.554	1347.893	2436.176	398.275	2239.254	-29.991
4000	764.940	1991.910	1363.753	2512.629	395.836	2286.547	-29.859
4100	765.711	2010.808	1379.305	2589.162	393.123	2333.849	-29.733
4200	766.430	2029.269	1394.562	2665.770	390.157	2381.214	-29.614
4300	767.102	2047.311	1409.533	2742.447	386.926	2428.587	-29.501
4400	767.730	2064.954	1424.229	2819.189	383.438	2476.105	-29.395
4500	768.319	2082.213	1438.660	2895.991	379.702	2523.748	-29.294
4600	768.871	2099.106	1452.834	2972.851	375.682	2571.481	-29.199
4700	769.390	2115.647	1466.761	3049.765	371.387	2619.221	-29.109
4800	769.878	2131.851	1480.449	3126.728	366.853	2667.133	-29.024
4900	770.338	2147.730	1493.906	3203.739	362.024	2715.043	-28.942
5000	770.771	2163.297	1507.138	3280.795	356.970	2763.193	-28.866

3.67. Cyclopenta[hi]chrysene



Other names: Benz[j]acephenanthrylene

Formula: C₂₀H₁₂

Mass: 252.309 g/mol

CAS Number: 216-48-8

Point Group: C_s

Length: 13.79 Å

Width: 9.108 Å

Breadth: 3.884 Å

L/B Ratio: 1.514

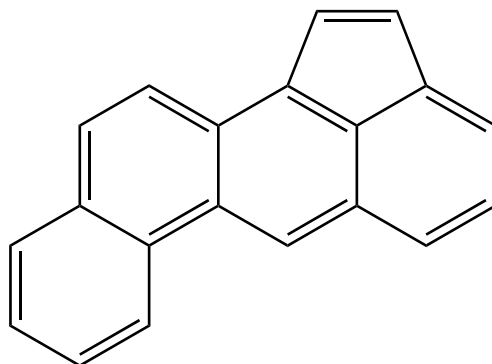
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C	-2.6256	2.4263	0.0000	C	0.0496	-0.8991	0.0000	H	-5.3371	-0.8599	0.0000
C	-3.7956	1.7290	0.0000	C	0.8529	-2.0779	0.0000	H	-4.1387	-3.0316	0.0000
C	-3.5067	0.2842	0.0000	C	2.2091	-1.9970	0.0000	H	-1.6538	-3.1634	0.0000
C	-4.2432	-0.8727	0.0000	C	2.0882	0.4566	0.0000	H	0.3822	2.5475	0.0000
C	-3.5473	-2.1093	0.0000	C	2.8572	-0.7230	0.0000	H	0.3312	-3.0462	0.0000
C	-2.1708	-2.1941	0.0000	C	4.2710	-0.6401	0.0000	H	2.8280	-2.9016	0.0000
C	-1.4930	1.4837	0.0000	C	4.8954	0.5818	0.0000	H	4.8573	-1.5662	0.0000
C	-2.0880	0.1775	0.0000	C	4.1311	1.7651	0.0000	H	5.9882	0.6481	0.0000
C	-1.3861	-1.0129	0.0000	C	2.7603	1.7040	0.0000	H	4.6419	2.7336	0.0000
C	-0.1381	1.5785	0.0000	H	-2.5034	3.5075	0.0000	H	2.1582	2.6252	0.0000
C	0.6486	0.3707	0.0000	H	-4.8047	2.1364	0.0000				

Table 3.67: Table of thermodynamic data as a function of temperature for Cyclopenta[hi]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			$\log K_f$
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-37.679	393.012	393.012	∞
100	82.695	314.158	637.081	-32.292	413.348	444.272	-232.059
200	161.160	394.066	495.650	-20.317	402.639	479.448	-125.216
250	207.739	434.987	479.404	-11.104	397.556	499.239	-104.308
298.15	253.408	475.489	475.489	0.000	393.012	519.246	-90.968
300	255.144	477.062	475.494	0.470	392.844	520.028	-90.543
350	300.799	519.856	478.769	14.380	388.640	541.567	-80.823
400	343.137	562.828	486.592	30.495	384.972	563.664	-73.605
450	381.472	605.498	497.438	48.627	381.779	586.195	-68.042
500	415.722	647.498	510.351	68.573	378.993	609.076	-63.628
600	473.137	728.576	540.025	113.131	374.417	655.544	-57.069
700	518.559	805.054	572.480	162.802	371.000	702.689	-52.434
800	555.029	876.764	606.083	216.545	368.605	750.240	-48.985
900	584.797	943.913	639.930	273.585	367.101	798.032	-46.316
1000	609.431	1006.842	673.508	333.334	366.366	845.960	-44.187
1100	630.036	1065.922	706.525	395.337	366.255	893.936	-42.449
1200	647.418	1121.508	738.814	459.234	366.664	941.886	-40.998
1300	662.184	1173.928	770.287	524.734	367.458	989.793	-39.770
1400	674.806	1223.475	800.904	591.599	368.539	1037.631	-38.714
1500	685.656	1270.412	830.654	659.636	369.848	1085.385	-37.796
1600	695.031	1314.969	859.543	728.681	371.287	1133.039	-36.989
1700	703.172	1357.355	887.590	798.601	372.803	1180.583	-36.274
1800	710.274	1397.753	914.819	869.281	374.339	1228.085	-35.637
1900	716.499	1436.326	941.259	940.627	375.873	1275.462	-35.064
2000	721.979	1473.220	966.942	1012.556	377.362	1322.779	-34.547
2100	726.822	1508.565	991.898	1085.001	378.751	1370.012	-34.076
2200	731.121	1542.478	1016.158	1157.903	380.038	1417.185	-33.648
2300	734.949	1575.063	1039.755	1231.210	381.220	1464.300	-33.255
2400	738.372	1606.416	1062.717	1304.879	382.243	1511.332	-32.893
2500	741.443	1636.622	1085.073	1378.872	383.116	1558.408	-32.560
2600	744.207	1665.756	1106.850	1453.157	383.813	1605.365	-32.252
2700	746.702	1693.890	1128.074	1527.705	384.337	1652.353	-31.966
2800	748.961	1721.088	1148.770	1602.490	384.668	1699.341	-31.701
2900	751.013	1747.406	1168.961	1677.490	384.784	1746.282	-31.453
3000	752.881	1772.899	1188.670	1752.686	384.718	1793.241	-31.222
3100	754.587	1797.614	1207.917	1828.061	384.413	1840.149	-31.006
3200	756.147	1821.596	1226.721	1903.599	383.899	1887.125	-30.804
3300	757.579	1844.886	1245.102	1979.286	383.162	1934.149	-30.614
3400	758.895	1867.522	1263.077	2055.111	382.183	1981.136	-30.436
3500	760.107	1889.538	1280.663	2131.062	380.964	2028.141	-30.268
3600	761.226	1910.967	1297.875	2207.129	379.521	2075.248	-30.110
3700	762.261	1931.838	1314.729	2283.304	377.832	2122.412	-29.962
3800	763.220	1952.179	1331.237	2359.579	375.877	2169.580	-29.822
3900	764.111	1972.016	1347.414	2435.946	373.686	2216.765	-29.690
4000	764.939	1991.372	1363.272	2512.399	371.247	2264.112	-29.566
4100	765.710	2010.270	1378.823	2588.932	368.534	2311.468	-29.448
4200	766.429	2028.730	1394.078	2665.539	365.567	2358.886	-29.336
4300	767.101	2046.773	1409.048	2742.216	362.336	2406.313	-29.230
4400	767.729	2064.415	1423.743	2818.958	358.848	2453.885	-29.131
4500	768.318	2081.675	1438.173	2895.761	355.113	2501.582	-29.037
4600	768.871	2098.568	1452.346	2972.620	351.092	2549.369	-28.948
4700	769.389	2115.109	1466.272	3049.534	346.798	2597.163	-28.864
4800	769.877	2131.312	1479.959	3126.497	342.263	2645.129	-28.784
4900	770.337	2147.191	1493.414	3203.508	337.434	2693.092	-28.708
5000	770.770	2162.759	1506.646	3280.564	332.380	2741.296	-28.638

3.68. Benz[*j*]aceanthrylene



Other names: Indeno[1,7*a-a*]phenanthrene
Cholanthrylene
Naphth[2,1-*d*]acenaphthylene

Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 202-33-5
Point Group: C_s

Length: 13.77 Å
Width: 9.075 Å
Breadth: 3.884 Å
L/B Ratio: 1.517

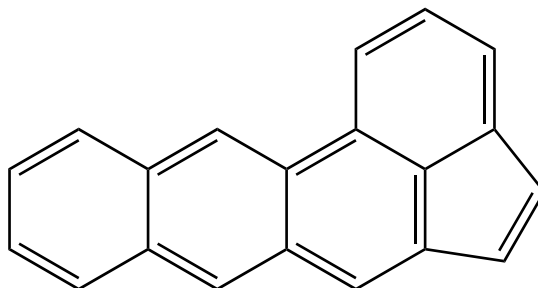
Cartesian coordinates:

C	-2.6994	-1.6682	0.0000	C	2.0785	0.0349	0.0000	H	2.2316	-3.3452	0.0000
C	-2.0891	-0.3993	0.0000	C	1.5808	-1.2637	0.0000	H	4.6406	-2.7909	0.0000
C	-2.9065	0.7445	0.0000	C	0.1773	-1.3875	0.0000	H	5.4603	-0.4539	0.0000
C	-4.3070	0.6047	0.0000	C	2.5634	-2.3016	0.0000	H	-0.2821	-2.3883	0.0000
C	-4.8831	-0.6490	0.0000	C	3.8976	-1.9856	0.0000	H	-0.5116	3.2069	0.0000
C	-4.0735	-1.7916	0.0000	C	4.3822	-0.6409	0.0000	H	-2.9808	2.9264	0.0000
C	-2.3116	2.0581	0.0000	C	3.4712	0.3738	0.0000	H	-4.9359	1.5024	0.0000
C	-0.9711	2.2115	0.0000	C	3.5124	1.8457	0.0000	H	-5.9727	-0.7561	0.0000
C	-0.0920	1.0707	0.0000	C	2.2386	2.3312	0.0000	H	-4.5363	-2.7838	0.0000
C	-0.6392	-0.2570	0.0000	H	1.9330	3.3760	0.0000	H	-2.0589	-2.5633	0.0000
C	1.2868	1.2077	0.0000	H	4.4365	2.4199	0.0000				

Table 3.68: Table of thermodynamic data as a function of temperature for Benz[*j*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-37.801	408.302	408.302	∞
100	82.913	315.309	639.061	-32.375	428.555	459.364	-239.942
200	161.614	395.440	497.271	-20.366	417.880	494.415	-129.125
250	208.252	436.470	480.986	-11.129	412.821	514.134	-107.420
298.15	253.921	477.063	477.063	0.000	408.302	534.067	-93.564
300	255.656	478.639	477.068	0.471	408.136	534.846	-93.123
350	301.281	521.510	480.349	14.406	403.957	556.305	-83.022
400	343.576	564.544	488.185	30.543	400.312	578.317	-75.519
450	381.868	607.262	499.047	48.697	397.139	600.761	-69.733
500	416.079	649.302	511.978	68.662	394.372	623.553	-65.141
600	473.431	730.439	541.687	113.252	389.828	669.838	-58.313
700	518.808	806.959	574.174	162.950	386.438	716.794	-53.487
800	555.246	878.700	607.805	216.716	384.067	764.153	-49.893
900	584.990	945.873	641.677	273.776	382.583	811.750	-47.112
1000	609.604	1008.822	675.278	333.544	381.866	859.480	-44.894
1100	630.192	1067.917	708.314	395.563	381.772	907.258	-43.081
1200	647.560	1123.517	740.621	459.475	382.195	955.007	-41.570
1300	662.314	1175.947	772.110	524.988	383.003	1002.714	-40.289
1400	674.925	1225.504	802.742	591.866	384.097	1050.349	-39.188
1500	685.765	1272.447	832.505	659.914	385.417	1097.900	-38.231
1600	695.131	1317.012	861.405	728.970	386.867	1145.350	-37.391
1700	703.264	1359.404	889.463	798.899	388.392	1192.690	-36.646
1800	710.359	1399.807	916.702	869.589	389.937	1239.986	-35.983
1900	716.578	1438.384	943.151	940.942	391.478	1287.158	-35.386
2000	722.052	1475.282	968.842	1012.879	392.976	1334.268	-34.847
2100	726.890	1510.630	993.806	1085.331	394.372	1381.296	-34.357
2200	731.184	1544.546	1018.074	1158.239	395.666	1428.262	-33.911
2300	735.008	1577.135	1041.677	1231.552	396.853	1475.170	-33.501
2400	738.427	1608.490	1064.645	1305.227	397.882	1521.994	-33.125
2500	741.494	1638.697	1087.007	1379.226	398.760	1568.863	-32.779
2600	744.255	1667.834	1108.789	1453.516	399.462	1615.613	-32.457
2700	746.747	1695.970	1130.019	1528.068	399.990	1662.392	-32.160
2800	749.004	1723.169	1150.719	1602.857	400.326	1709.173	-31.884
2900	751.053	1749.488	1170.915	1677.862	400.446	1755.905	-31.627
3000	752.919	1774.982	1190.628	1753.062	400.384	1802.656	-31.386
3100	754.622	1799.698	1209.879	1828.440	400.083	1849.356	-31.161
3200	756.181	1823.682	1228.687	1903.982	399.572	1896.123	-30.950
3300	757.611	1846.973	1247.072	1979.672	398.838	1942.939	-30.754
3400	758.925	1869.610	1265.051	2055.500	397.862	1989.716	-30.568
3500	760.136	1891.627	1282.640	2131.454	396.646	2036.513	-30.393
3600	761.253	1913.056	1299.855	2207.524	395.206	2083.411	-30.229
3700	762.287	1933.928	1316.711	2283.702	393.520	2130.366	-30.075
3800	763.245	1954.270	1333.223	2359.979	391.567	2177.325	-29.929
3900	764.134	1974.107	1349.402	2436.348	389.379	2224.301	-29.791
4000	764.961	1993.464	1365.263	2512.804	386.942	2271.439	-29.661
4100	765.731	2012.362	1380.816	2589.339	384.231	2318.585	-29.539
4200	766.449	2030.823	1396.074	2665.948	381.266	2365.795	-29.422
4300	767.120	2048.866	1411.046	2742.627	378.037	2413.012	-29.312
4400	767.748	2066.509	1425.743	2819.371	374.551	2460.375	-29.208
4500	768.336	2083.769	1440.175	2896.175	370.817	2507.862	-29.110
4600	768.888	2100.663	1454.350	2973.037	366.799	2555.440	-29.017
4700	769.406	2117.204	1468.278	3049.951	362.506	2603.024	-28.929
4800	769.893	2133.408	1481.967	3126.917	357.973	2650.780	-28.846
4900	770.352	2149.287	1495.424	3203.929	353.146	2698.534	-28.766
5000	770.785	2164.855	1508.658	3280.986	348.093	2746.529	-28.692

3.69. Benz[*k*]acephenanthrylene



Other names: Naphth[2,3-*e*]acenaphthylene

Formula: C₂₀H₁₂

Mass: 252.309 g/mol

CAS Number: 212-41-9

Point Group: C_s

Length: 13.97 Å

Width: 9.125 Å

Breadth: 3.883 Å

L/B Ratio: 1.531

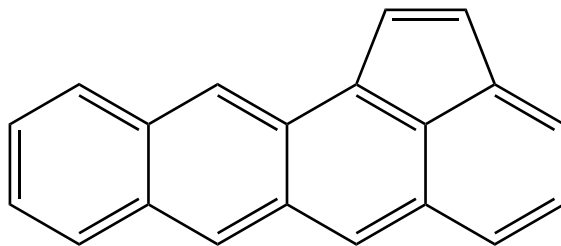
Cartesian coordinates:

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C	-4.3705	0.9727	0.0000	C	1.2374	-1.1292	0.0000	H	-3.1988	-3.6501	0.0000
C	-3.6331	-0.3025	0.0000	C	1.5536	1.6541	0.0000	H	-0.8077	-2.9990	0.0000
C	-3.9742	-1.6368	0.0000	C	2.6926	0.8258	0.0000	H	-0.6942	3.0913	0.0000
C	-2.9320	-2.5875	0.0000	C	2.5338	-0.5794	0.0000	H	1.1088	-2.2210	0.0000
C	-1.5926	-2.2321	0.0000	C	3.6933	-1.4108	0.0000	H	1.6894	2.7432	0.0000
C	-2.1118	1.4810	0.0000	C	4.9395	-0.8551	0.0000	H	3.5603	-2.4985	0.0000
C	-2.2592	0.0404	0.0000	C	5.0994	0.5556	0.0000	H	5.8330	-1.4880	0.0000
C	-1.2215	-0.8713	0.0000	C	4.0093	1.3760	0.0000	H	6.1119	0.9724	0.0000
C	-0.8705	2.0101	0.0000	H	-3.7188	3.0719	0.0000	H	4.1240	2.4659	0.0000
C	0.2765	1.1139	0.0000	H	-5.4570	1.0336	0.0000				

Table 3.69: Table of thermodynamic data as a function of temperature for Benz[*k*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-37.715	394.656	394.656	∞
100	82.424	314.247	637.675	-32.343	414.941	445.857	-232.887
200	161.447	394.141	495.972	-20.366	404.234	481.028	-125.629
250	208.258	435.152	479.685	-11.133	399.171	500.813	-104.637
298.15	254.081	475.759	475.759	0.000	394.656	520.809	-91.242
300	255.821	477.337	475.764	0.472	394.490	521.591	-90.815
350	301.561	520.242	479.048	14.418	390.322	543.114	-81.054
400	343.927	563.318	486.891	30.571	386.693	565.188	-73.804
450	382.256	606.081	497.763	48.743	383.539	587.693	-68.216
500	416.482	648.162	510.706	68.728	380.792	610.542	-63.782
600	473.832	729.373	540.443	113.358	376.288	656.937	-57.190
700	519.193	805.954	572.960	163.095	372.937	703.997	-52.532
800	555.614	877.745	606.621	216.900	370.603	751.454	-49.064
900	585.339	944.960	640.521	273.996	369.156	799.145	-46.380
1000	609.936	1007.945	674.148	333.797	368.473	846.964	-44.240
1100	630.506	1067.071	707.208	395.849	368.411	894.828	-42.491
1200	647.856	1122.697	739.538	459.791	368.865	942.661	-41.032
1300	662.592	1175.151	771.048	525.333	369.701	990.448	-39.796
1400	675.185	1224.727	801.700	592.238	370.822	1038.162	-38.733
1500	686.008	1271.688	831.481	660.311	372.167	1085.789	-37.810
1600	695.358	1316.268	860.399	729.391	373.641	1133.315	-36.998
1700	703.475	1358.673	888.472	799.342	375.188	1180.728	-36.279
1800	710.556	1399.087	915.726	870.051	376.753	1228.097	-35.638
1900	716.762	1437.675	942.189	941.424	378.314	1275.340	-35.061
2000	722.223	1474.582	967.892	1013.379	379.829	1322.521	-34.540
2100	727.050	1509.938	992.868	1085.847	381.241	1369.618	-34.067
2200	731.334	1543.862	1017.148	1158.771	382.551	1416.653	-33.635
2300	735.148	1576.456	1040.761	1232.098	383.752	1463.629	-33.239
2400	738.559	1607.817	1063.740	1305.787	384.795	1510.521	-32.875
2500	741.618	1638.030	1086.111	1379.798	385.686	1557.456	-32.541
2600	744.371	1667.171	1107.902	1454.100	386.400	1604.273	-32.230
2700	746.856	1695.312	1129.140	1528.664	386.940	1651.119	-31.942
2800	749.107	1722.514	1149.849	1603.464	387.286	1697.965	-31.675
2900	751.150	1748.838	1170.052	1678.478	387.416	1744.762	-31.426
3000	753.011	1774.335	1189.772	1753.688	387.364	1791.578	-31.193
3100	754.709	1799.054	1209.030	1829.075	387.071	1838.342	-30.975
3200	756.263	1823.040	1227.845	1904.625	386.569	1885.174	-30.772
3300	757.689	1846.333	1246.235	1980.323	385.843	1932.054	-30.581
3400	758.999	1868.972	1264.220	2056.159	384.874	1978.895	-30.401
3500	760.206	1890.992	1281.815	2132.120	383.665	2025.755	-30.232
3600	761.320	1912.423	1299.035	2208.197	382.233	2072.717	-30.074
3700	762.351	1933.297	1315.896	2284.381	380.553	2119.735	-29.925
3800	763.306	1953.640	1332.413	2360.664	378.606	2166.757	-29.784
3900	764.192	1973.479	1348.597	2437.040	376.424	2213.796	-29.650
4000	765.016	1992.837	1364.462	2513.501	373.993	2260.996	-29.525
4100	765.784	2011.737	1380.020	2590.041	371.287	2308.205	-29.406
4200	766.500	2030.199	1395.281	2666.656	368.328	2355.477	-29.294
4300	767.169	2048.243	1410.257	2743.339	365.103	2402.757	-29.187
4400	767.794	2065.887	1424.958	2820.088	361.622	2450.182	-29.087
4500	768.381	2083.148	1439.393	2896.897	357.893	2497.731	-28.992
4600	768.931	2100.043	1453.572	2973.763	353.879	2545.371	-28.903
4700	769.447	2116.585	1467.504	3050.682	349.590	2593.017	-28.818
4800	769.933	2132.790	1481.196	3127.651	345.061	2640.836	-28.738
4900	770.390	2148.670	1494.656	3204.668	340.238	2688.652	-28.661
5000	770.821	2164.238	1507.893	3281.728	335.188	2736.707	-28.590

3.70. Cyclopenta[de]naphthacene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 16683-64-0
Point Group: C_s

Length: 14.08 Å
Width: 8.582 Å
Breadth: 3.884 Å
L/B Ratio: 1.641

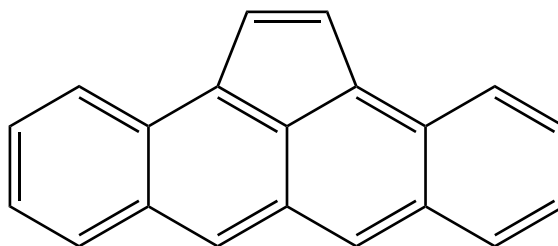
Cartesian coordinates:

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C	-2.7215	-0.7673	0.0000	C	2.1248	-1.2678	0.0000	H	5.5145	-1.7788	0.0000
C	-2.6045	0.6572	0.0000	C	0.8514	-1.8176	0.0000	H	5.5810	0.6948	0.0000
C	-3.8047	1.4501	0.0000	C	3.3916	-1.9516	0.0000	H	0.7187	-2.9060	0.0000
C	-5.0246	0.8574	0.0000	C	4.5577	-1.2448	0.0000	H	-1.2502	2.3378	0.0000
C	-5.1422	-0.5681	0.0000	C	4.6084	0.1933	0.0000	H	-1.6777	-2.6487	0.0000
C	-1.3504	1.2453	0.0000	C	3.4381	0.8803	0.0000	H	-3.7039	2.5414	0.0000
C	-0.1856	0.4542	0.0000	C	3.0309	2.2946	0.0000	H	-5.9411	1.4564	0.0000
C	-0.2938	-0.9772	0.0000	C	1.6682	2.3655	0.0000	H	-6.1444	-1.0088	0.0000
C	-1.5827	-1.5554	0.0000	H	1.0558	3.2653	0.0000	H	-4.1162	-2.4455	0.0000
C	1.1114	1.0048	0.0000	H	3.7351	3.1235	0.0000				

Table 3.70: Table of thermodynamic data as a function of temperature for Cyclopenta[de]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-37.897	435.800	435.800	∞
100	82.708	314.078	639.310	-32.523	455.905	486.837	-254.292
200	162.416	394.372	496.796	-20.485	445.259	522.007	-136.331
250	209.492	435.630	480.416	-11.196	440.251	541.774	-113.195
298.15	255.447	476.468	476.468	0.000	435.800	561.742	-98.413
300	257.190	478.054	476.473	0.474	435.636	562.522	-97.942
350	302.967	521.174	479.774	14.490	431.538	584.003	-87.156
400	345.310	564.437	487.654	30.713	427.979	606.026	-79.137
450	383.581	607.359	498.575	48.953	424.893	628.471	-72.950
500	417.733	649.576	511.572	69.002	422.210	651.253	-68.035
600	474.921	731.001	541.419	113.749	417.823	697.496	-60.721
700	520.128	807.738	574.041	163.588	414.574	744.384	-55.545
800	556.415	879.645	607.797	217.479	412.326	791.656	-51.689
900	586.028	946.948	641.783	274.649	410.953	839.153	-48.702
1000	610.531	1010.000	675.486	334.514	410.334	886.770	-46.319
1100	631.024	1069.179	708.614	396.622	410.328	934.426	-44.371
1200	648.309	1124.848	741.004	460.613	410.830	982.045	-42.746
1300	662.992	1177.335	772.568	526.197	411.709	1029.615	-41.370
1400	675.539	1226.940	803.268	593.140	412.868	1077.109	-40.187
1500	686.324	1273.924	833.093	661.246	414.246	1124.514	-39.158
1600	695.641	1318.523	862.051	730.356	415.750	1171.815	-38.255
1700	703.730	1360.944	890.160	800.334	417.323	1219.002	-37.455
1800	710.787	1401.373	917.446	871.067	418.913	1266.143	-36.742
1900	716.971	1439.972	943.940	942.462	420.496	1313.157	-36.100
2000	722.415	1476.889	969.671	1014.437	422.031	1360.108	-35.522
2100	727.225	1512.255	994.672	1086.924	423.462	1406.974	-34.996
2200	731.494	1546.186	1018.975	1159.864	424.788	1453.777	-34.516
2300	735.297	1578.788	1042.611	1233.207	426.005	1500.520	-34.077
2400	738.696	1610.155	1065.609	1306.910	427.062	1547.179	-33.673
2500	741.745	1640.373	1087.999	1380.935	427.966	1593.880	-33.302
2600	744.489	1669.519	1109.808	1455.249	428.692	1640.462	-32.957
2700	746.966	1697.663	1131.062	1529.824	429.243	1687.073	-32.638
2800	749.209	1724.870	1151.786	1604.634	429.600	1733.684	-32.342
2900	751.246	1751.197	1172.004	1679.658	429.740	1780.245	-32.065
3000	753.101	1776.697	1191.738	1754.877	429.697	1826.825	-31.807
3100	754.794	1801.419	1211.008	1830.273	429.413	1873.353	-31.565
3200	756.343	1825.407	1229.835	1905.831	428.919	1919.948	-31.339
3300	757.764	1848.703	1248.237	1981.537	428.201	1966.591	-31.128
3400	759.070	1871.345	1266.233	2057.380	427.240	2013.195	-30.928
3500	760.273	1893.366	1283.838	2133.348	426.038	2059.818	-30.740
3600	761.384	1914.799	1301.068	2209.432	424.611	2106.542	-30.564
3700	762.411	1935.674	1317.939	2285.622	422.938	2153.323	-30.399
3800	763.363	1956.019	1334.464	2361.911	420.997	2200.106	-30.242
3900	764.246	1975.860	1350.656	2438.292	418.820	2246.908	-30.093
4000	765.068	1995.219	1366.529	2514.758	416.394	2293.870	-29.954
4100	765.833	2014.120	1382.095	2591.304	413.694	2340.841	-29.822
4200	766.547	2032.584	1397.364	2667.923	410.739	2387.874	-29.697
4300	767.214	2050.629	1412.347	2744.612	407.520	2434.915	-29.578
4400	767.837	2068.274	1427.055	2821.365	404.042	2482.102	-29.466
4500	768.422	2085.536	1441.496	2898.178	400.318	2529.412	-29.360
4600	768.970	2102.431	1455.681	2975.048	396.308	2576.813	-29.260
4700	769.485	2118.974	1469.619	3051.971	392.023	2624.221	-29.164
4800	769.969	2135.180	1483.316	3128.944	387.497	2671.800	-29.075
4900	770.425	2151.061	1496.782	3205.964	382.677	2719.377	-28.988
5000	770.855	2166.630	1510.024	3283.028	377.632	2767.194	-28.908

3.71. Benz[*d*]aceanthrylene



Other names: Cyclopenta[*fg*]naphthacene

Formula: C₂₀H₁₂

Mass: 252.309 g/mol

CAS Number: 19770-52-6

Point Group: C_{2v}

Length: 14.08 Å

Width: 8.585 Å

Breadth: 3.883 Å

L/B Ratio: 1.640

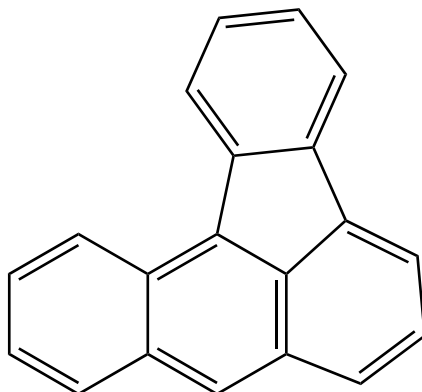
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C	-2.4021	-0.4581	0.0000	C	2.4019	-0.4592	0.0000	H	1.3337	2.8450	0.0000
C	-2.4309	0.9822	0.0000	C	1.1646	-1.0813	0.0000	H	3.5935	-2.2793	0.0000
C	-3.7175	1.6282	0.0000	C	3.6398	-1.1842	0.0000	H	5.7740	-1.0751	0.0000
C	-4.8649	0.9046	0.0000	C	4.8266	-0.5262	0.0000	H	5.8417	1.3978	0.0000
C	-4.8269	-0.5240	0.0000	C	4.8653	0.9023	0.0000	H	3.7466	2.7224	0.0000
C	-1.2690	1.7509	0.0000	C	3.7182	1.6265	0.0000	H	-3.7453	2.7242	0.0000
C	0.0003	1.1299	0.0000	C	-0.6833	-2.4687	0.0000	H	-5.8411	1.4005	0.0000
C	-0.0001	-0.2692	0.0000	C	0.6822	-2.4690	0.0000	H	-5.7746	-1.0724	0.0000
C	-1.1651	-1.0807	0.0000	H	1.3406	-3.3355	0.0000	H	-3.5945	-2.2776	0.0000
C	1.2698	1.7503	0.0000	H	-1.3421	-3.3348	0.0000				

Table 3.71: Table of thermodynamic data as a function of temperature for Benz[*d*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-37.857	434.145	434.145	∞
100	82.899	306.557	631.845	-32.529	454.245	485.929	-253.818
200	162.502	387.033	489.357	-20.465	443.625	521.840	-136.288
250	209.272	428.277	472.996	-11.180	438.614	541.974	-113.237
298.15	254.988	469.055	469.055	0.000	434.145	562.298	-98.510
300	256.723	470.638	469.060	0.473	433.981	563.092	-98.041
350	302.341	513.673	472.355	14.462	429.855	584.946	-87.297
400	344.601	556.846	480.219	30.651	426.262	607.346	-79.310
450	382.841	599.683	491.118	48.854	423.140	630.173	-73.147
500	416.994	641.822	504.088	68.867	420.420	653.340	-68.253
600	474.230	723.116	533.879	113.542	415.961	700.365	-60.971
700	519.506	799.751	566.445	163.315	412.646	748.047	-55.819
800	555.859	871.580	600.146	217.147	410.340	796.123	-51.980
900	585.532	938.821	634.082	274.265	408.914	844.429	-49.008
1000	610.087	1001.823	667.740	334.083	408.248	892.861	-46.637
1100	630.625	1060.962	700.827	396.148	408.200	941.337	-44.699
1200	647.950	1116.597	733.180	460.101	408.665	989.780	-43.083
1300	662.666	1169.058	764.710	525.652	409.509	1038.176	-41.714
1400	675.244	1218.639	795.380	592.563	410.637	1086.499	-40.537
1500	686.055	1265.604	825.176	660.642	411.987	1134.735	-39.514
1600	695.396	1310.186	854.108	729.725	413.465	1182.869	-38.616
1700	703.506	1352.593	882.194	799.680	415.015	1230.890	-37.820
1800	710.581	1393.010	909.458	870.392	416.583	1278.867	-37.111
1900	716.782	1431.598	935.932	941.767	418.146	1326.718	-36.473
2000	722.240	1468.506	961.644	1013.724	419.663	1374.507	-35.898
2100	727.064	1503.864	986.628	1086.194	421.077	1422.211	-35.375
2200	731.345	1537.787	1010.915	1159.119	422.388	1469.853	-34.898
2300	735.158	1570.383	1034.536	1232.447	423.591	1517.437	-34.461
2400	738.567	1601.744	1057.520	1306.137	424.634	1564.936	-34.059
2500	741.624	1631.957	1079.897	1380.149	425.526	1612.479	-33.690
2600	744.376	1661.098	1101.694	1454.451	426.241	1659.903	-33.347
2700	746.861	1689.239	1122.937	1529.015	426.781	1707.356	-33.030
2800	749.110	1716.442	1143.650	1603.816	427.127	1754.809	-32.736
2900	751.153	1742.765	1163.858	1678.830	427.258	1802.214	-32.461
3000	753.013	1768.262	1183.582	1754.040	427.206	1849.637	-32.204
3100	754.711	1792.982	1202.844	1829.428	426.913	1897.009	-31.964
3200	756.265	1816.968	1221.662	1904.978	426.411	1944.448	-31.739
3300	757.690	1840.261	1240.056	1980.676	425.686	1991.934	-31.529
3400	759.000	1862.900	1258.044	2056.512	424.717	2039.383	-31.331
3500	760.207	1884.919	1275.641	2132.473	423.508	2086.850	-31.144
3600	761.321	1906.351	1292.865	2208.550	422.075	2134.419	-30.969
3700	762.351	1927.225	1309.729	2284.734	420.396	2182.045	-30.804
3800	763.306	1947.568	1326.248	2361.018	418.449	2229.674	-30.648
3900	764.192	1967.407	1342.434	2437.393	416.267	2277.320	-30.501
4000	765.016	1986.765	1358.301	2513.854	413.836	2325.127	-30.362
4100	765.784	2005.665	1373.861	2590.395	411.130	2372.944	-30.231
4200	766.500	2024.127	1389.125	2667.009	408.171	2420.823	-30.107
4300	767.169	2042.171	1404.103	2743.693	404.946	2468.710	-29.988
4400	767.794	2059.815	1418.806	2820.442	401.465	2516.742	-29.877
4500	768.380	2077.076	1433.243	2897.251	397.736	2564.898	-29.772
4600	768.930	2093.971	1447.424	2974.116	393.722	2613.146	-29.673
4700	769.447	2110.513	1461.356	3051.036	389.433	2661.399	-29.578
4800	769.933	2126.718	1475.050	3128.005	384.904	2709.825	-29.488
4900	770.390	2142.598	1488.512	3205.021	380.080	2758.248	-29.403
5000	770.821	2158.166	1501.750	3282.082	375.031	2806.911	-29.323

3.72. Benz[*a*]aceanthrylene



Other names: Benzo[*a*]fluoranthene
 Dibenzo[*c,lm*]fluorene
 Naphtho[3,2,1-*jk*]fluorene
 1,9-Phenyleneanthracene

Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 203-33-8
Point Group: C_s

Length: 12.52 Å
Width: 10.78 Å
Breadth: 3.885 Å
L/B Ratio: 1.162

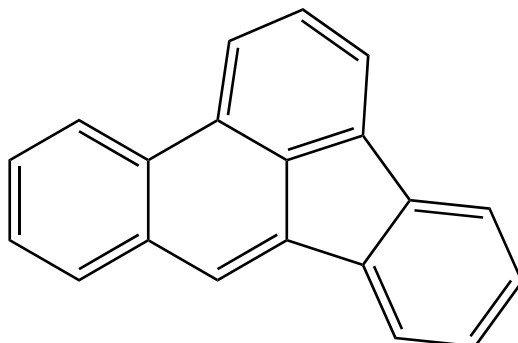
Cartesian coordinates:

C	3.0358	-2.5997	0.0000	C	0.0853	-0.3486	0.0000	H	4.6133	0.4365	0.0000
C	4.0858	-1.6362	0.0000	C	-0.1409	1.0416	0.0000	H	0.9077	-2.9278	0.0000
C	3.8063	-0.3055	0.0000	C	-1.5471	1.3527	0.0000	H	3.0188	2.2575	0.0000
C	1.7358	-2.2014	0.0000	C	-1.2415	-0.9784	0.0000	H	1.1758	4.1697	0.0000
C	1.4011	-0.8103	0.0000	C	-2.2332	0.0545	0.0000	H	-1.2371	4.7119	0.0000
C	2.4505	0.1644	0.0000	C	-3.5762	-0.2622	0.0000	H	-2.9839	2.9526	0.0000
C	2.1875	1.5426	0.0000	C	-3.9404	-1.6145	0.0000	H	-4.3380	0.5237	0.0000
C	0.8677	2.0103	0.0000	C	-2.9799	-2.6163	0.0000	H	-5.0023	-1.8818	0.0000
C	0.4235	3.3736	0.0000	C	-1.6150	-2.3077	0.0000	H	-3.2910	-3.6662	0.0000
C	-0.9116	3.6657	0.0000	H	3.2972	-3.6629	0.0000	H	-0.8477	-3.0954	0.0000
C	-1.9300	2.6579	0.0000	H	5.1219	-1.9902	0.0000				

Table 3.72: Table of thermodynamic data as a function of temperature for Benz[*a*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-37.698	373.844	373.844	∞
100	83.199	313.430	636.547	-32.312	394.161	425.158	-222.075
200	161.292	393.628	495.110	-20.297	383.492	460.389	-120.239
250	207.510	434.538	478.885	-11.087	378.406	480.201	-100.330
298.15	252.923	474.976	474.976	0.000	373.844	500.231	-87.637
300	254.652	476.546	474.981	0.470	373.676	501.015	-87.233
350	300.157	519.252	478.250	14.351	369.443	522.581	-77.989
400	342.430	562.133	486.056	30.431	365.741	544.710	-71.130
450	380.756	604.718	496.880	48.528	362.512	567.279	-65.847
500	415.030	646.644	509.766	68.439	359.691	590.200	-61.657
600	472.545	727.604	539.385	112.931	355.050	636.760	-55.434
700	518.085	804.000	571.787	162.549	351.579	684.007	-51.040
800	554.666	875.654	605.341	216.251	349.143	731.666	-47.772
900	584.528	942.766	639.145	273.259	347.607	779.572	-45.244
1000	609.236	1005.670	672.686	332.985	346.849	827.615	-43.229
1100	629.899	1064.735	705.669	394.972	346.722	875.709	-41.583
1200	647.325	1120.311	737.930	458.857	347.119	923.778	-40.210
1300	662.125	1172.725	769.379	524.349	347.906	971.806	-39.047
1400	674.772	1222.269	799.975	591.210	348.983	1019.764	-38.047
1500	685.640	1269.203	829.707	659.244	350.289	1067.639	-37.178
1600	695.028	1313.760	858.579	728.289	351.728	1115.414	-36.414
1700	703.178	1356.146	886.612	798.209	353.243	1163.079	-35.736
1800	710.288	1396.545	913.828	868.890	354.781	1210.701	-35.133
1900	716.518	1435.118	940.257	940.237	356.316	1258.199	-34.590
2000	722.001	1472.013	965.929	1012.169	357.807	1305.637	-34.099
2100	726.847	1507.360	990.876	1084.616	359.199	1352.991	-33.653
2200	731.147	1541.274	1015.128	1157.520	360.489	1400.284	-33.246
2300	734.976	1573.861	1038.717	1230.830	361.672	1447.520	-32.874
2400	738.400	1605.215	1061.672	1304.502	362.698	1494.671	-32.530
2500	741.470	1635.421	1084.022	1378.498	363.575	1541.867	-32.215
2600	744.234	1664.557	1105.793	1452.786	364.274	1588.945	-31.922
2700	746.728	1692.692	1127.012	1527.336	364.800	1636.053	-31.651
2800	748.987	1719.890	1147.703	1602.124	365.134	1683.161	-31.399
2900	751.039	1746.209	1167.890	1677.126	365.253	1730.221	-31.164
3000	752.906	1771.703	1187.594	1752.325	365.190	1777.300	-30.945
3100	754.611	1796.419	1206.837	1827.702	364.887	1824.328	-30.739
3200	756.171	1820.401	1225.638	1903.242	364.375	1871.423	-30.547
3300	757.601	1843.692	1244.016	1978.932	363.641	1918.567	-30.368
3400	758.917	1866.329	1261.988	2054.759	362.663	1965.672	-30.198
3500	760.128	1888.346	1279.571	2130.712	361.446	2012.797	-30.039
3600	761.247	1909.775	1296.780	2206.781	360.006	2060.023	-29.890
3700	762.281	1930.647	1313.631	2282.958	358.319	2107.307	-29.749
3800	763.239	1950.988	1330.137	2359.235	356.365	2154.593	-29.616
3900	764.129	1970.825	1346.311	2435.604	354.176	2201.898	-29.491
4000	764.956	1990.182	1362.167	2512.059	351.739	2249.363	-29.373
4100	765.726	2009.080	1377.716	2588.593	349.028	2296.838	-29.261
4200	766.445	2027.541	1392.969	2665.202	346.063	2344.376	-29.156
4300	767.116	2045.584	1407.937	2741.881	342.833	2391.921	-29.055
4400	767.744	2063.227	1422.630	2818.624	339.347	2439.612	-28.961
4500	768.333	2080.487	1437.058	2895.428	335.613	2487.428	-28.873
4600	768.885	2097.380	1451.230	2972.289	331.594	2535.334	-28.789
4700	769.403	2113.922	1465.155	3049.204	327.301	2583.246	-28.709
4800	769.891	2130.125	1478.840	3126.169	322.768	2631.331	-28.634
4900	770.350	2146.005	1492.294	3203.181	317.940	2679.413	-28.562
5000	770.782	2161.572	1505.525	3280.238	312.887	2727.736	-28.496

3.73. Benz[*e*]acephenanthrylene



Other names: 3,4-Benz[*e*]acephenanthrylene
Benzo[*b*]fluoranthene
Benzo[*e*]fluoranthene
2,3-Benzofluoranthene
3,4-Benzofluoranthene

Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 205-99-2
Point Group: C_s

Length: 13.75 Å
Width: 9.906 Å
Breadth: 3.884 Å
L/B Ratio: 1.388

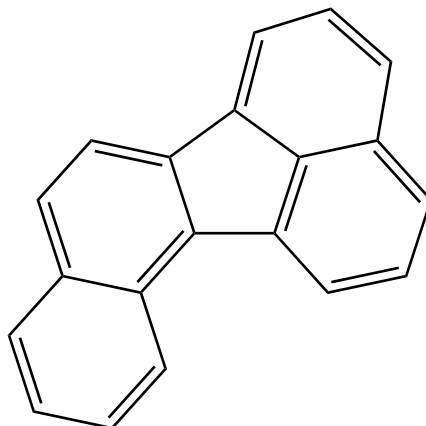
Cartesian coordinates:

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C	-1.8833	0.9703	0.0000	C	1.1136	-1.1296	0.0000	H	-4.2560	-1.5217	0.0000
C	-2.6968	2.0847	0.0000	C	0.6203	1.7171	0.0000	H	-2.1705	-3.3220	0.0000
C	-4.0844	1.8946	0.0000	C	1.9669	1.1878	0.0000	H	0.0775	-4.3813	0.0000
C	-4.6332	0.6206	0.0000	C	2.2241	-0.2030	0.0000	H	2.1609	-3.0254	0.0000
C	-3.8183	-0.5185	0.0000	C	3.5540	-0.6656	0.0000	H	0.4724	2.8027	0.0000
C	-1.3556	-1.3244	0.0000	C	4.6037	0.2263	0.0000	H	3.7290	-1.7505	0.0000
C	-1.2731	-2.6956	0.0000	C	4.3539	1.6072	0.0000	H	5.6367	-0.1363	0.0000
C	0.0116	-3.2877	0.0000	C	3.0601	2.0804	0.0000	H	5.1962	2.3068	0.0000
C	1.1745	-2.5427	0.0000	H	-2.2686	3.0920	0.0000	H	2.8681	3.1597	0.0000
C	-0.4194	0.8498	0.0000	H	-4.7434	2.7692	0.0000				

Table 3.73: Table of thermodynamic data as a function of temperature for Benz[*e*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-37.574	342.578	342.578	∞
100	83.339	313.192	635.143	-32.195	363.011	394.032	-205.817
200	160.596	393.230	494.270	-20.208	352.314	429.291	-112.117
250	206.582	433.957	478.115	-11.040	347.187	449.128	-93.838
298.15	251.911	474.223	474.223	0.000	342.578	469.190	-82.198
300	253.638	475.786	474.228	0.468	342.408	469.975	-81.828
350	299.146	518.335	477.484	14.298	338.124	491.584	-73.363
400	341.467	561.084	485.263	30.329	334.373	513.762	-67.089
450	379.861	603.560	496.052	48.379	331.097	536.385	-62.261
500	414.212	645.395	508.901	68.247	328.234	559.367	-58.435
600	471.875	726.219	538.444	112.665	323.518	606.059	-52.761
700	517.546	802.522	570.775	162.223	319.987	653.449	-48.760
800	554.236	874.112	604.266	215.876	317.503	701.260	-45.787
900	584.185	941.178	638.016	272.846	315.928	749.322	-43.489
1000	608.962	1004.050	671.509	332.541	315.140	797.526	-41.658
1100	629.680	1063.091	704.451	394.503	314.988	845.783	-40.162
1200	647.149	1118.650	736.676	458.369	315.366	894.017	-38.915
1300	661.982	1171.051	768.093	523.845	316.136	942.212	-37.858
1400	674.655	1220.585	798.661	590.694	317.200	990.338	-36.949
1500	685.543	1267.512	828.367	658.717	318.495	1038.381	-36.159
1600	694.947	1312.064	857.218	727.753	319.925	1086.326	-35.464
1700	703.111	1354.445	885.230	797.665	321.434	1134.161	-34.848
1800	710.231	1394.840	912.429	868.340	322.965	1181.953	-34.299
1900	716.470	1433.411	938.841	939.682	324.494	1229.622	-33.804
2000	721.960	1470.304	964.499	1011.609	325.982	1277.230	-33.357
2100	726.811	1505.648	989.432	1084.053	327.369	1324.756	-32.951
2200	731.116	1539.561	1013.673	1156.953	328.656	1372.220	-32.580
2300	734.949	1572.146	1037.250	1230.260	329.837	1419.627	-32.240
2400	738.376	1603.499	1060.195	1303.930	330.860	1466.950	-31.927
2500	741.449	1633.704	1082.535	1377.924	331.734	1514.318	-31.639
2600	744.215	1662.839	1104.297	1452.209	332.432	1561.568	-31.372
2700	746.712	1690.974	1125.508	1526.758	332.956	1608.847	-31.124
2800	748.973	1718.172	1146.192	1601.544	333.288	1656.127	-30.895
2900	751.025	1744.490	1166.371	1676.545	333.406	1703.359	-30.680
3000	752.894	1769.983	1186.069	1751.743	333.341	1750.609	-30.480
3100	754.600	1794.699	1205.306	1827.119	333.037	1797.809	-30.292
3200	756.161	1818.681	1224.101	1902.658	332.524	1845.077	-30.117
3300	757.592	1841.972	1242.473	1978.346	331.789	1892.392	-29.953
3400	758.908	1864.608	1260.440	2054.172	330.811	1939.670	-29.799
3500	760.121	1886.625	1278.018	2130.125	329.593	1986.967	-29.653
3600	761.240	1908.054	1295.222	2206.193	328.152	2034.365	-29.517
3700	762.274	1928.925	1312.069	2282.370	326.464	2081.821	-29.389
3800	763.233	1949.267	1328.571	2358.646	324.510	2129.279	-29.268
3900	764.123	1969.104	1344.741	2435.014	322.320	2176.756	-29.154
4000	764.951	1988.460	1360.593	2511.468	319.883	2224.394	-29.047
4100	765.722	2007.358	1376.138	2588.002	317.171	2272.041	-28.946
4200	766.441	2025.819	1391.388	2664.611	314.205	2319.751	-28.850
4300	767.112	2043.862	1406.353	2741.289	310.975	2367.468	-28.758
4400	767.740	2061.505	1421.043	2818.032	307.488	2415.332	-28.673
4500	768.329	2078.765	1435.468	2894.836	303.754	2463.319	-28.593
4600	768.881	2095.658	1449.637	2971.696	299.735	2511.397	-28.517
4700	769.400	2112.199	1463.559	3048.611	295.441	2559.482	-28.445
4800	769.888	2128.403	1477.241	3125.575	290.908	2607.739	-28.377
4900	770.347	2144.282	1490.693	3202.587	286.080	2655.994	-28.313
5000	770.780	2159.850	1503.921	3279.644	281.026	2704.488	-28.253

3.74. Benzo[*j*]fluoranthene



Other names: 7,8-Benzfluoranthene
Benzo[*l*]fluoranthene
10,11-Benzofluoranthene
Dibenzo[*a,jk*]fluorene

Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 205-82-3
Point Group: C_s

Length: 13.26 Å
Width: 9.565 Å
Breadth: 3.888 Å
L/B Ratio: 1.386

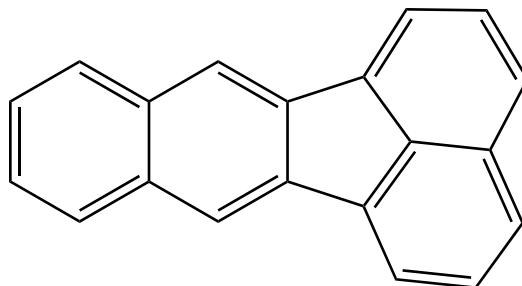
Cartesian coordinates:

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C	-3.1640	-2.1219	0.0000	C	2.1615	2.2664	0.0000	H	-2.3782	3.1943	0.0000
C	-2.0193	-2.8838	0.0000	C	0.7977	2.4473	0.0000	H	-4.6950	2.3076	0.0000
C	-0.7148	-2.3168	0.0000	C	2.7324	0.9677	0.0000	H	-5.1737	-0.1187	0.0000
C	-1.7932	-0.1711	0.0000	C	1.9045	-0.1819	0.0000	H	2.8312	3.1341	0.0000
C	-1.4986	1.2274	0.0000	C	2.5022	-1.4734	0.0000	H	0.3544	3.4483	0.0000
C	-2.5410	2.1120	0.0000	C	3.8620	-1.6045	0.0000	H	1.8417	-2.3548	0.0000
C	-3.8660	1.5911	0.0000	C	4.6930	-0.4570	0.0000	H	4.3263	-2.5961	0.0000
C	-4.1404	0.2441	0.0000	C	4.1462	0.7954	0.0000	H	5.7798	-0.5900	0.0000
C	-3.0758	-0.7013	0.0000	H	-4.1524	-2.5936	0.0000	H	4.7853	1.6858	0.0000
C	-0.0315	1.3175	0.0000	H	-2.1007	-3.9764	0.0000				

Table 3.74: Table of thermodynamic data as a function of temperature for Benzo[*j*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-37.719	362.378	362.378	∞
100	83.365	315.575	638.158	-32.258	382.748	413.531	-216.002
200	160.947	395.645	496.967	-20.264	372.058	448.551	-117.147
250	207.183	436.481	480.766	-11.071	366.955	468.265	-97.837
298.15	252.610	476.863	476.863	0.000	362.378	488.203	-85.529
300	254.338	478.431	476.868	0.469	362.209	488.982	-85.138
350	299.852	521.089	480.133	14.335	357.961	510.456	-76.180
400	342.136	563.930	487.930	30.400	354.244	532.494	-69.535
450	380.478	606.481	498.743	48.482	351.000	554.974	-64.418
500	414.772	648.379	511.619	68.380	348.166	577.808	-60.362
600	472.329	729.296	541.214	112.849	343.501	624.197	-54.340
700	517.907	805.661	573.594	162.447	340.011	671.275	-50.090
800	554.521	877.294	607.128	216.132	337.559	718.770	-46.930
900	584.409	944.390	640.915	273.128	336.010	766.512	-44.486
1000	609.138	1007.283	674.440	332.843	335.241	814.394	-42.539
1100	629.818	1066.339	707.411	394.821	335.105	862.327	-40.948
1200	647.257	1121.909	739.660	458.698	335.495	910.236	-39.621
1300	662.067	1174.317	771.099	524.184	336.274	958.104	-38.496
1400	674.722	1223.857	801.686	591.040	337.346	1005.903	-37.530
1500	685.596	1270.788	831.409	659.070	338.648	1053.619	-36.690
1600	694.990	1315.343	860.274	728.110	340.082	1101.236	-35.951
1700	703.145	1357.727	888.299	798.026	341.594	1148.743	-35.296
1800	710.259	1398.123	915.510	868.704	343.129	1196.208	-34.712
1900	716.492	1436.696	941.933	940.049	344.661	1243.548	-34.187
2000	721.978	1473.589	967.600	1011.978	346.150	1290.828	-33.712
2100	726.826	1508.934	992.542	1084.423	347.539	1338.024	-33.281
2200	731.127	1542.848	1016.791	1157.325	348.827	1385.160	-32.887
2300	734.959	1575.434	1040.376	1230.633	350.009	1432.238	-32.526
2400	738.384	1606.787	1063.327	1304.303	351.033	1479.233	-32.194
2500	741.456	1636.993	1085.673	1378.298	351.908	1526.272	-31.889
2600	744.220	1666.128	1107.442	1452.584	352.606	1573.192	-31.605
2700	746.716	1694.262	1128.658	1527.133	353.131	1620.143	-31.343
2800	748.976	1721.460	1149.346	1601.919	353.463	1667.094	-31.099
2900	751.028	1747.779	1169.531	1676.921	353.581	1713.997	-30.872
3000	752.896	1773.272	1189.233	1752.119	353.517	1760.918	-30.660
3100	754.601	1797.988	1208.473	1827.495	353.213	1807.790	-30.460
3200	756.162	1821.970	1227.272	1903.034	352.700	1854.728	-30.275
3300	757.593	1845.261	1245.648	1978.723	351.965	1901.715	-30.101
3400	758.909	1867.897	1263.618	2054.549	350.987	1948.664	-29.937
3500	760.121	1889.914	1281.199	2130.501	349.770	1995.631	-29.783
3600	761.240	1911.343	1298.407	2206.570	348.328	2042.701	-29.638
3700	762.274	1932.214	1315.256	2282.747	346.641	2089.827	-29.502
3800	763.233	1952.556	1331.760	2359.023	344.687	2136.957	-29.374
3900	764.123	1972.393	1347.934	2435.391	342.497	2184.105	-29.252
4000	764.951	1991.749	1363.788	2511.845	340.059	2231.414	-29.139
4100	765.721	2010.648	1379.336	2588.379	337.347	2278.732	-29.031
4200	766.440	2029.108	1394.587	2664.988	334.382	2326.113	-28.929
4300	767.112	2047.151	1409.554	2741.666	331.152	2373.501	-28.832
4400	767.740	2064.794	1424.246	2818.409	327.665	2421.036	-28.741
4500	768.329	2082.054	1438.673	2895.212	323.930	2468.695	-28.655
4600	768.881	2098.947	1452.844	2972.073	319.911	2516.444	-28.575
4700	769.399	2115.488	1466.767	3048.987	315.617	2564.200	-28.497
4800	769.887	2131.692	1480.452	3125.952	311.084	2612.128	-28.425
4900	770.346	2147.571	1493.905	3202.964	306.256	2660.054	-28.356
5000	770.779	2163.139	1507.135	3280.020	301.202	2708.219	-28.292

3.75. Benzo[*k*]fluoranthene



Other names: 11,12-Benzofluoranthene
8,9-Benzofluoranthene
2,3:1',8'-Binaphthylene
Dibenzo[*b,jk*]fluorene

Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 207-08-9
Point Group: C_{2v}

Length: 13.54 Å
Width: 9.195 Å
Breadth: 3.885 Å
L/B Ratio: 1.473

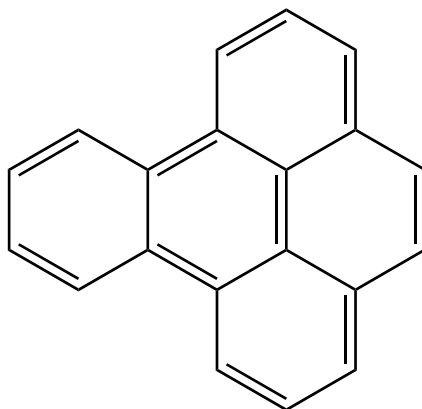
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C	-3.0437	-2.6891	0.0000	C	1.2260	1.5374	0.0000	H	-4.0317	3.0661	0.0000
C	-1.6277	-2.5456	0.0000	C	2.5172	0.9235	0.0000	H	-5.2140	0.8930	0.0000
C	-2.0026	-0.1710	0.0000	C	2.6373	-0.4834	0.0000	H	1.5729	-2.3979	0.0000
C	-1.3062	1.0765	0.0000	C	3.9291	-1.0679	0.0000	H	1.1434	2.6298	0.0000
C	-2.0357	2.2328	0.0000	C	5.0491	-0.2770	0.0000	H	4.0165	-2.1604	0.0000
C	-3.4556	2.1342	0.0000	C	4.9291	1.1288	0.0000	H	6.0470	-0.7277	0.0000
C	-4.1196	0.9310	0.0000	C	3.6913	1.7185	0.0000	H	5.8361	1.7421	0.0000
C	-3.3865	-0.2891	0.0000	H	-4.9871	-1.7641	0.0000	H	3.5921	2.8099	0.0000
C	0.1233	0.7404	0.0000	H	-3.4535	-3.7052	0.0000				

Table 3.75: Table of thermodynamic data as a function of temperature for Benzo[*k*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-37.575	349.432	349.432	∞
100	82.648	308.340	630.282	-32.194	369.866	401.372	-209.651
200	160.623	388.043	489.298	-20.251	359.125	437.139	-114.167
250	207.057	428.827	473.104	-11.069	354.011	457.234	-95.532
298.15	252.648	469.202	469.202	0.000	349.432	477.541	-83.661
300	254.382	470.770	469.206	0.469	349.263	478.334	-83.284
350	300.011	513.444	472.472	14.340	345.020	500.191	-74.648
400	342.359	556.311	480.274	30.415	341.313	522.611	-68.245
450	380.730	598.891	491.092	48.509	338.081	545.471	-63.315
500	415.034	640.815	503.975	68.420	335.260	568.683	-59.409
600	472.588	721.779	533.588	112.915	330.621	615.826	-53.611
700	518.162	798.184	565.986	162.539	327.156	663.655	-49.521
800	554.773	869.851	599.539	216.249	324.729	711.895	-46.481
900	584.661	936.977	633.344	273.270	323.206	760.380	-44.130
1000	609.388	999.896	666.886	333.010	322.462	809.002	-42.257
1100	630.063	1058.976	699.873	395.013	322.351	857.673	-40.727
1200	647.495	1114.567	732.138	458.915	322.765	906.317	-39.450
1300	662.297	1166.994	763.591	524.424	323.568	954.918	-38.368
1400	674.942	1216.551	794.192	591.302	324.662	1003.449	-37.438
1500	685.806	1263.497	823.928	659.353	325.985	1051.894	-36.629
1600	695.189	1308.064	852.805	728.414	327.440	1100.240	-35.918
1700	703.332	1350.460	880.842	798.350	328.972	1148.474	-35.288
1800	710.435	1390.867	908.063	869.046	330.524	1196.665	-34.726
1900	716.658	1429.448	934.497	940.408	332.073	1244.730	-34.219
2000	722.134	1466.350	960.174	1012.353	333.579	1292.734	-33.762
2100	726.973	1501.703	985.125	1084.813	334.983	1340.654	-33.346
2200	731.266	1535.623	1009.382	1157.729	336.285	1388.513	-32.967
2300	735.089	1568.215	1032.975	1231.051	337.480	1436.313	-32.619
2400	738.506	1599.573	1055.934	1304.733	338.517	1484.029	-32.298
2500	741.571	1629.784	1078.288	1378.740	339.404	1531.789	-32.004
2600	744.329	1658.924	1100.063	1453.037	340.113	1579.431	-31.730
2700	746.819	1687.062	1121.286	1527.597	340.649	1627.101	-31.478
2800	749.073	1714.264	1141.980	1602.393	340.991	1674.772	-31.243
2900	751.120	1740.586	1162.171	1677.405	341.118	1722.395	-31.023
3000	752.983	1766.082	1181.878	1752.611	341.063	1770.035	-30.818
3100	754.684	1790.800	1201.124	1827.996	340.768	1817.626	-30.626
3200	756.240	1814.785	1219.928	1903.543	340.263	1865.283	-30.447
3300	757.667	1838.078	1238.309	1979.239	339.535	1912.988	-30.279
3400	758.979	1860.717	1256.284	2055.073	338.565	1960.655	-30.121
3500	760.188	1882.735	1273.869	2131.032	337.354	2008.340	-29.972
3600	761.304	1904.166	1291.081	2207.107	335.919	2056.128	-29.833
3700	762.335	1925.039	1307.934	2283.290	334.238	2103.972	-29.702
3800	763.291	1945.382	1324.443	2359.572	332.290	2151.819	-29.578
3900	764.179	1965.221	1340.619	2435.946	330.106	2199.684	-29.461
4000	765.004	1984.579	1356.477	2512.405	327.673	2247.710	-29.351
4100	765.772	2003.478	1372.028	2588.945	324.966	2295.745	-29.248
4200	766.489	2021.940	1387.284	2665.558	322.006	2343.843	-29.149
4300	767.158	2039.984	1402.254	2742.241	318.781	2391.948	-29.056
4400	767.785	2057.628	1416.949	2818.988	315.298	2440.200	-28.968
4500	768.371	2074.889	1431.379	2895.796	311.568	2488.575	-28.886
4600	768.922	2091.783	1445.552	2972.661	307.553	2537.040	-28.808
4700	769.439	2108.325	1459.478	3049.580	303.264	2585.513	-28.734
4800	769.925	2124.530	1473.165	3126.548	298.734	2634.157	-28.665
4900	770.383	2140.410	1486.621	3203.564	293.910	2682.799	-28.598
5000	770.814	2155.978	1499.853	3280.624	288.860	2731.681	-28.537

3.76. Benzo[e]pyrene



Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 192-97-2
Point Group: C_{2v}

Length: 11.67 Å
Width: 10.42 Å
Breadth: 3.886 Å
L/B Ratio: 1.120

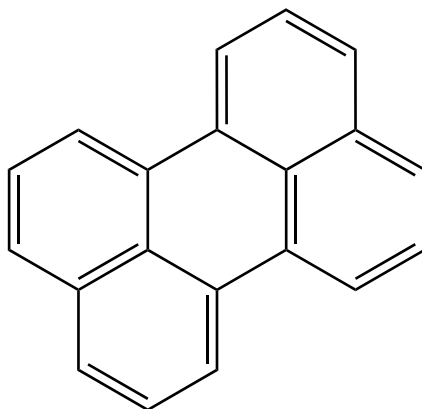
Cartesian coordinates:

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C	2.8018	1.4670	0.0000	C	0.4021	-2.8188	0.0000	H	-4.2943	1.1220	0.0000
C	2.8792	-1.3087	0.0000	C	-0.8821	0.6941	0.0000	H	-4.2251	-1.3595	0.0000
C	1.6342	-0.6577	0.0000	C	-2.1657	2.7607	0.0000	H	-2.9464	-3.4439	0.0000
C	1.5950	0.7476	0.0000	C	-2.1264	1.3579	0.0000	H	-0.7639	-4.6320	0.0000
C	-3.3396	0.5836	0.0000	C	-0.9886	3.4878	0.0000	H	1.3670	-3.3487	0.0000
C	-3.3019	-0.7687	0.0000	C	0.2444	2.8368	0.0000	H	-3.1336	3.2745	0.0000
C	0.3963	-1.4258	0.0000	C	0.3162	1.4457	0.0000	H	-1.0206	4.5823	0.0000
C	-0.8420	-0.7422	0.0000	H	5.0210	-1.1047	0.0000	H	1.1782	3.4197	0.0000
C	-2.0474	-1.4743	0.0000	H	4.9516	1.3827	0.0000				

Table 3.76: Table of thermodynamic data as a function of temperature for Benzo[*e*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-37.007	299.819	299.819	∞
100	79.637	305.343	623.010	-31.767	320.680	352.486	-184.116
200	158.736	383.352	483.655	-20.061	309.702	388.654	-101.504
250	205.132	423.716	467.608	-10.973	304.494	408.995	-85.453
298.15	250.568	463.738	463.738	0.000	299.819	429.556	-75.255
300	252.297	465.294	463.743	0.465	299.646	430.360	-74.931
350	297.824	507.637	466.983	14.229	295.296	452.499	-67.530
400	340.165	550.211	474.726	30.194	291.479	475.217	-62.056
450	378.601	592.536	485.469	48.180	288.139	498.388	-57.850
500	413.011	634.241	498.267	67.987	285.214	521.924	-54.524
600	470.810	714.858	527.706	112.292	280.385	569.743	-49.599
700	516.609	791.007	559.937	161.749	276.754	618.277	-46.135
800	553.405	862.478	593.335	215.314	274.181	667.245	-43.566
900	583.441	929.452	627.001	272.206	272.528	716.475	-41.582
1000	608.292	992.250	660.420	331.830	271.669	765.855	-40.003
1100	629.071	1051.229	693.294	393.728	271.453	815.296	-38.714
1200	646.594	1106.738	725.458	457.536	271.773	864.719	-37.639
1300	661.475	1159.097	756.820	522.959	272.490	914.107	-36.729
1400	674.191	1208.595	787.338	589.759	273.506	963.430	-35.945
1500	685.118	1255.491	816.999	657.738	274.757	1012.674	-35.264
1600	694.556	1300.016	845.808	726.733	276.146	1061.822	-34.664
1700	702.751	1342.375	873.782	796.608	277.617	1110.863	-34.132
1800	709.899	1382.750	900.946	867.248	279.113	1159.864	-33.658
1900	716.162	1421.304	927.326	938.558	280.611	1208.742	-33.230
2000	721.675	1458.181	952.953	1010.456	282.069	1257.562	-32.843
2100	726.547	1493.512	977.859	1082.872	283.429	1306.300	-32.492
2200	730.870	1527.413	1002.073	1155.747	284.690	1354.979	-32.171
2300	734.720	1559.988	1025.627	1229.030	285.847	1403.601	-31.876
2400	738.162	1591.331	1048.549	1302.677	286.848	1452.141	-31.604
2500	741.249	1621.528	1070.868	1376.651	287.701	1500.726	-31.355
2600	744.028	1650.656	1092.611	1450.917	288.380	1549.193	-31.123
2700	746.536	1678.783	1113.803	1525.447	288.886	1597.691	-30.909
2800	748.807	1705.975	1134.469	1600.216	289.201	1646.190	-30.709
2900	750.870	1732.288	1154.632	1675.202	289.303	1694.642	-30.523
3000	752.747	1757.776	1174.315	1750.384	289.223	1743.113	-30.350
3100	754.461	1782.487	1193.537	1825.746	288.905	1791.534	-30.187
3200	756.030	1806.465	1212.318	1901.271	288.378	1840.023	-30.035
3300	757.469	1829.752	1230.677	1976.947	287.630	1888.560	-29.893
3400	758.791	1852.384	1248.631	2052.761	286.640	1937.060	-29.759
3500	760.009	1874.398	1266.197	2128.702	285.411	1985.580	-29.633
3600	761.134	1895.824	1283.390	2204.760	283.959	2034.201	-29.515
3700	762.174	1916.692	1300.226	2280.926	282.261	2082.880	-29.404
3800	763.137	1937.031	1316.717	2357.192	280.297	2131.562	-29.300
3900	764.032	1956.866	1332.878	2433.551	278.098	2180.262	-29.201
4000	764.864	1976.220	1348.721	2509.996	275.651	2229.124	-29.109
4100	765.638	1995.116	1364.257	2586.522	272.931	2277.995	-29.021
4200	766.361	2013.575	1379.498	2663.122	269.957	2326.929	-28.939
4300	767.036	2031.616	1394.455	2739.793	266.720	2375.871	-28.861
4400	767.668	2049.257	1409.137	2816.528	263.225	2424.959	-28.787
4500	768.259	2066.515	1423.554	2893.325	259.484	2474.172	-28.719
4600	768.814	2083.407	1437.716	2970.179	255.458	2523.475	-28.654
4700	769.335	2099.947	1451.630	3047.087	251.157	2572.785	-28.593
4800	769.826	2116.149	1465.306	3124.045	246.618	2622.267	-28.535
4900	770.287	2132.027	1478.751	3201.051	241.784	2671.747	-28.481
5000	770.722	2147.593	1491.973	3278.101	236.724	2721.467	-28.430

3.77. Perylene



Other names: Dibenz[*de,kl*]anthracene
peri-Dinaphthalene

Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 198-55-0
Point Group: D_{2h}

Length: 11.68 Å
Width: 9.170 Å
Breadth: 3.884 Å
L/B Ratio: 1.274

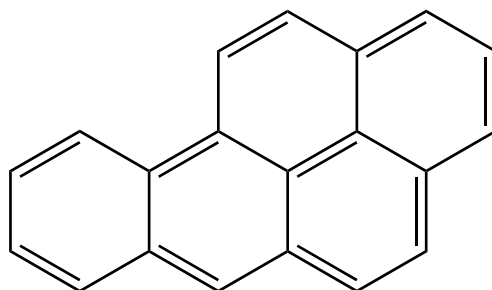
Cartesian coordinates:

C	0.7351	-1.2421	0.0000	C	-3.5381	-1.2466	0.0000	H	4.6423	-1.2052	0.0000
C	1.4539	-2.4196	0.0000	C	-2.8463	-2.4283	0.0000	H	-0.9156	3.3801	0.0000
C	2.8630	-2.4087	0.0000	C	-1.4373	-2.4295	0.0000	H	-3.4018	3.3619	0.0000
C	3.5466	-1.2222	0.0000	C	1.4287	0.0049	0.0000	H	-4.6423	1.2052	0.0000
C	-0.7351	1.2420	0.0000	C	2.8401	0.0098	0.0000	H	-4.6339	-1.2371	0.0000
C	-1.4539	2.4196	0.0000	C	3.5381	1.2465	0.0000	H	-3.3786	-3.3852	0.0000
C	-2.8630	2.4087	0.0000	C	2.8463	2.4283	0.0000	H	-0.8923	-3.3862	0.0000
C	-3.5465	1.2222	0.0000	C	1.4373	2.4295	0.0000	H	4.6339	1.2371	0.0000
C	-0.7266	-1.2471	0.0000	C	0.7266	1.2471	0.0000	H	3.3786	3.3852	0.0000
C	-1.4287	-0.0049	0.0000	H	0.9156	-3.3801	0.0000	H	0.8924	3.3863	0.0000
C	-2.8401	-0.0098	0.0000	H	3.4018	-3.3619	0.0000				

Table 3.77: Table of thermodynamic data as a function of temperature for Perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-37.184	329.131	329.131	∞
100	80.173	302.528	621.328	-31.880	340.148	372.235	-194.432
200	159.296	380.926	481.515	-20.118	329.226	408.663	-106.730
250	205.714	421.418	465.424	-11.002	324.046	429.122	-89.658
298.15	251.175	461.545	461.545	0.000	319.400	449.791	-78.800
300	252.904	463.104	461.550	0.466	319.228	450.599	-78.455
350	298.447	505.543	464.797	14.261	314.909	472.845	-70.567
400	340.789	548.200	472.557	30.257	311.123	495.666	-64.726
450	379.213	590.597	483.321	48.274	307.814	518.936	-60.235
500	413.601	632.366	496.144	68.111	304.919	542.567	-56.680
600	471.345	713.086	525.632	112.472	300.146	590.568	-51.412
700	517.085	789.312	557.912	161.980	296.566	639.275	-47.702
800	553.827	860.844	591.356	215.590	294.038	688.409	-44.948
900	583.817	927.865	625.063	272.521	292.425	737.801	-42.820
1000	608.627	990.700	658.518	332.181	291.601	787.338	-41.125
1100	629.371	1049.710	691.427	394.111	291.417	836.932	-39.742
1200	646.864	1105.243	723.620	457.948	291.766	886.506	-38.588
1300	661.719	1157.623	755.010	523.396	292.508	936.042	-37.610
1400	674.411	1207.138	785.553	590.219	293.547	985.512	-36.769
1500	685.318	1254.049	815.236	658.219	294.819	1034.900	-36.038
1600	694.739	1298.586	844.065	727.233	296.227	1084.192	-35.395
1700	702.917	1340.955	872.058	797.126	297.716	1133.375	-34.824
1800	710.051	1381.340	899.238	867.782	299.228	1182.518	-34.315
1900	716.303	1419.901	925.635	939.107	300.741	1231.537	-33.857
2000	721.804	1456.786	951.277	1011.018	302.212	1280.497	-33.442
2100	726.666	1492.123	976.196	1083.446	303.584	1329.374	-33.066
2200	730.980	1526.029	1000.423	1156.333	304.857	1378.191	-32.722
2300	734.823	1558.608	1023.988	1229.626	306.024	1426.952	-32.406
2400	738.257	1589.956	1046.921	1303.284	307.036	1475.629	-32.116
2500	741.338	1620.157	1069.250	1377.266	307.898	1524.351	-31.849
2600	744.111	1649.288	1091.003	1451.541	308.585	1572.956	-31.600
2700	746.614	1677.418	1112.204	1526.079	309.099	1621.590	-31.371
2800	748.880	1704.612	1132.878	1600.856	309.422	1670.226	-31.158
2900	750.938	1730.928	1153.049	1675.848	309.530	1718.814	-30.959
3000	752.812	1756.418	1172.739	1751.037	309.457	1767.421	-30.773
3100	754.522	1781.131	1191.968	1826.405	309.145	1815.978	-30.598
3200	756.087	1805.111	1210.756	1901.937	308.625	1864.602	-30.436
3300	757.523	1828.400	1229.121	1977.619	307.883	1913.274	-30.284
3400	758.842	1851.034	1247.081	2053.438	306.898	1961.910	-30.140
3500	760.058	1873.049	1264.653	2129.384	305.674	2010.564	-30.005
3600	761.180	1894.476	1281.852	2205.446	304.226	2059.320	-29.879
3700	762.218	1915.346	1298.693	2281.617	302.533	2108.133	-29.761
3800	763.179	1935.686	1315.189	2357.887	300.573	2156.950	-29.649
3900	764.072	1955.521	1331.355	2434.250	298.378	2205.785	-29.543
4000	764.902	1974.877	1347.202	2510.699	295.935	2254.781	-29.444
4100	765.675	1993.774	1362.742	2587.229	293.219	2303.786	-29.350
4200	766.396	2012.233	1377.987	2663.833	290.249	2352.855	-29.261
4300	767.069	2030.275	1392.948	2740.506	287.014	2401.931	-29.177
4400	767.699	2047.917	1407.634	2817.245	283.523	2451.153	-29.098
4500	768.289	2065.176	1422.055	2894.045	279.785	2500.499	-29.024
4600	768.843	2082.068	1436.220	2970.902	275.762	2549.937	-28.955
4700	769.363	2098.609	1450.138	3047.812	271.464	2599.381	-28.888
4800	769.852	2114.812	1463.817	3124.773	266.927	2648.997	-28.826
4900	770.313	2130.690	1477.265	3201.782	262.096	2698.610	-28.767
5000	770.747	2146.257	1490.490	3278.835	257.039	2748.464	-28.712

3.78. Benzo[*a*]pyrene



Other names: Benzo[*def*]chrysene
3,4-Benzopyrene
6,7-Benzopyrene
1,2-Benzopyrene
4,5-Benzopyrene

Formula: C₂₀H₁₂
Mass: 252.309 g/mol
CAS Number: 50-32-8
Point Group: C_s

Length: 13.74 Å
Width: 9.197 Å
Breadth: 3.886 Å
L/B Ratio: 1.494

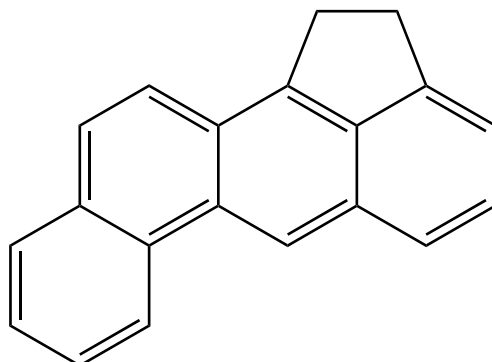
Cartesian coordinates:

C	4.3506	-1.2083	0.0000	C	-4.0099	0.6858	0.0000	H	4.1438	2.1988	0.0000
C	4.7622	0.1433	0.0000	C	-4.4348	-0.6461	0.0000	H	2.6800	-2.5717	0.0000
C	3.8323	1.1480	0.0000	C	-3.5181	-1.6799	0.0000	H	1.8218	2.9279	0.0000
C	3.0185	-1.5243	0.0000	C	0.6329	-0.8104	0.0000	H	-0.5133	3.6805	0.0000
C	2.0311	-0.5040	0.0000	C	-0.3003	0.2313	0.0000	H	-2.9353	3.1538	0.0000
C	2.4437	0.8449	0.0000	C	-1.7020	-0.0627	0.0000	H	-4.7506	1.4934	0.0000
C	1.4784	1.8859	0.0000	C	-2.1390	-1.4034	0.0000	H	-5.5074	-0.8672	0.0000
C	0.1342	1.5952	0.0000	C	-1.1621	-2.4524	0.0000	H	-3.8573	-2.7219	0.0000
C	-0.8657	2.6425	0.0000	C	0.1644	-2.1649	0.0000	H	-1.5134	-3.4905	0.0000
C	-2.1831	2.3565	0.0000	H	5.1090	-1.9979	0.0000	H	0.9227	-2.9632	0.0000
C	-2.6535	0.9887	0.0000	H	5.8322	0.3752	0.0000				

Table 3.78: Table of thermodynamic data as a function of temperature for Benzo[*a*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-37.080	305.905	305.905	∞
100	79.422	309.753	628.757	-31.900	317.628	348.993	-182.291
200	159.468	387.884	488.740	-20.171	306.673	384.718	-100.476
250	206.296	428.462	472.604	-11.035	301.513	404.827	-84.582
298.15	251.973	468.712	468.712	0.000	296.900	425.155	-74.484
300	253.707	470.276	468.717	0.468	296.730	425.949	-74.163
350	299.322	512.845	471.975	14.305	292.453	447.833	-66.834
400	341.651	555.619	479.757	30.345	288.711	470.285	-61.412
450	380.021	598.115	490.552	48.404	285.444	493.182	-57.246
500	414.343	639.966	503.407	68.279	282.587	516.435	-53.951
600	471.963	720.810	532.963	112.708	277.882	563.670	-49.071
700	517.612	797.124	565.305	162.273	274.359	611.599	-45.637
800	554.291	868.722	598.806	215.933	271.881	659.950	-43.089
900	584.234	935.794	632.563	272.908	270.312	708.550	-41.122
1000	609.008	998.671	666.064	332.608	269.528	757.292	-39.556
1100	629.723	1057.716	699.012	394.574	269.380	806.088	-38.277
1200	647.189	1113.279	731.243	458.444	269.762	854.859	-37.210
1300	662.020	1165.684	762.665	523.924	270.536	903.590	-36.306
1400	674.691	1215.220	793.237	590.776	271.604	952.253	-35.528
1500	685.577	1262.150	822.948	658.803	272.903	1000.833	-34.851
1600	694.979	1306.703	851.802	727.842	274.336	1049.313	-34.256
1700	703.141	1349.087	879.818	797.758	275.848	1097.684	-33.727
1800	710.259	1389.483	907.019	868.436	277.382	1146.013	-33.256
1900	716.496	1428.056	933.435	939.780	278.914	1194.217	-32.831
2000	721.984	1464.950	959.095	1011.710	280.404	1242.361	-32.446
2100	726.834	1500.295	984.030	1084.156	281.794	1290.421	-32.097
2200	731.137	1534.209	1008.273	1157.058	283.082	1338.421	-31.777
2300	734.969	1566.795	1031.853	1230.367	284.265	1386.363	-31.485
2400	738.395	1598.149	1054.799	1304.039	285.291	1434.221	-31.214
2500	741.467	1628.355	1077.141	1378.035	286.167	1482.124	-30.967
2600	744.232	1657.491	1098.905	1452.322	286.866	1529.909	-30.736
2700	746.728	1685.626	1120.118	1526.872	287.392	1577.722	-30.522
2800	748.987	1712.824	1140.803	1601.660	287.726	1625.537	-30.324
2900	751.039	1739.143	1160.984	1676.663	287.845	1673.304	-30.139
3000	752.907	1764.637	1180.683	1751.861	287.781	1721.089	-29.966
3100	754.612	1789.353	1199.921	1827.239	287.479	1768.824	-29.804
3200	756.173	1813.336	1218.717	1902.779	286.967	1816.626	-29.653
3300	757.604	1836.627	1237.091	1978.469	286.233	1864.476	-29.512
3400	758.919	1859.263	1255.058	2054.296	285.256	1912.288	-29.378
3500	760.131	1881.280	1272.637	2130.249	284.039	1960.119	-29.253
3600	761.249	1902.709	1289.843	2206.319	282.599	2008.052	-29.135
3700	762.284	1923.581	1306.690	2282.496	280.912	2056.042	-29.026
3800	763.242	1943.923	1323.193	2358.773	278.959	2104.035	-28.921
3900	764.132	1963.760	1339.365	2435.142	276.770	2152.046	-28.823
4000	764.959	1983.117	1355.217	2511.597	274.333	2200.218	-28.731
4100	765.729	2002.015	1370.763	2588.132	271.622	2248.400	-28.644
4200	766.448	2020.476	1386.014	2664.741	268.657	2296.644	-28.562
4300	767.119	2038.519	1400.979	2741.420	265.428	2344.896	-28.484
4400	767.747	2056.162	1415.670	2818.164	261.942	2393.294	-28.411
4500	768.336	2073.422	1430.096	2894.968	258.208	2441.815	-28.343
4600	768.887	2090.315	1444.265	2971.830	254.190	2490.428	-28.279
4700	769.406	2106.857	1458.188	3048.745	249.897	2539.047	-28.218
4800	769.893	2123.061	1471.871	3125.710	245.364	2587.838	-28.161
4900	770.352	2138.940	1485.323	3202.722	240.536	2636.627	-28.106
5000	770.785	2154.508	1498.552	3279.779	235.483	2685.656	-28.056

3.79. 1,2-Dihydrobenz[*j*]aceanthrylene



Other names: Cholanthrene
Formula: C₂₀H₁₄
Mass: 254.325 g/mol
CAS Number: 479-23-2
Point Group: C₁

Length: 13.80 Å
Width: 8.980 Å
Breadth: 4.225 Å
L/B Ratio: 1.537

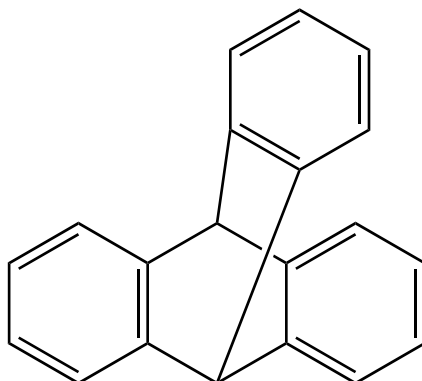
Cartesian coordinates:

C	-1.8238	2.5547	-0.1208	C	1.0364	2.2102	0.0164	H	-1.9848	-3.3088	-0.0167
C	-4.1004	1.6448	0.0298	C	2.3768	2.0485	0.0180	H	-4.4518	-2.9944	-0.0311
C	-3.5309	0.2768	0.0045	C	2.1352	-0.4014	0.0060	H	-5.4288	-0.7200	-0.0117
C	-2.4249	-2.3054	-0.0137	C	2.9645	0.7327	0.0121	H	0.2781	-2.3499	-0.0082
C	-3.7781	-2.1312	-0.0203	C	4.3634	0.5751	0.0104	H	0.5977	3.2156	0.0120
C	-4.3388	-0.8295	-0.0089	C	4.9215	-0.6865	0.0028	H	3.0503	2.9133	0.0230
C	-2.1069	0.1233	-0.0068	C	4.0976	-1.8198	-0.0035	H	5.0036	1.4646	0.0144
C	-1.2444	1.2516	-0.0036	C	2.7254	-1.6794	-0.0021	H	6.0095	-0.8084	0.0012
C	-0.1556	-1.3370	-0.0027	H	-1.7179	3.1655	0.7855	H	4.5487	-2.8173	-0.0098
C	-1.5522	-1.1763	-0.0055	H	-3.3832	2.4134	-0.4350	H	2.0677	-2.5622	-0.0077
C	0.6901	-0.2373	0.0058	H	-4.3297	1.9677	1.0527				
C	0.1448	1.0761	0.0147	H	-5.0173	1.7286	-0.5678				

Table 3.79: Table of thermodynamic data as a function of temperature for 1,2-Dihydrobenz[j]aceanthrylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-39.555	299.463	299.463	∞
100	89.272	321.554	659.262	-33.771	323.788	364.046	-190.154
200	168.401	406.258	511.758	-21.100	311.081	409.334	-106.905
250	215.639	448.855	494.900	-11.511	304.978	434.604	-90.804
298.15	262.501	490.843	490.843	0.000	299.463	460.082	-80.603
300	264.292	492.472	490.848	0.487	299.259	461.078	-80.279
350	311.663	536.801	494.241	14.896	294.105	488.465	-72.898
400	355.968	581.350	502.345	31.602	289.572	516.541	-67.452
450	396.352	625.649	513.589	50.427	285.610	545.154	-63.278
500	432.630	669.322	526.985	71.168	282.158	574.196	-59.985
600	493.864	753.826	557.809	117.611	276.537	633.160	-55.120
700	542.707	833.762	591.578	169.529	272.429	692.947	-51.707
800	582.202	908.898	626.597	225.841	269.651	753.217	-49.179
900	614.623	979.404	661.922	285.734	268.025	813.761	-47.228
1000	641.569	1045.598	697.014	348.584	267.387	874.441	-45.675
1100	664.181	1107.838	731.561	413.904	267.554	935.151	-44.406
1200	683.299	1166.471	765.385	481.304	268.388	995.803	-43.345
1300	699.566	1221.824	798.387	550.469	269.726	1056.371	-42.445
1400	713.487	1274.190	830.519	621.139	271.448	1116.826	-41.668
1500	725.463	1323.834	861.767	693.101	273.474	1177.146	-40.991
1600	735.816	1370.993	892.132	766.178	275.694	1237.318	-40.393
1700	744.810	1415.878	921.631	840.219	278.037	1297.328	-39.861
1800	752.658	1458.677	950.287	915.101	280.442	1357.247	-39.385
1900	759.539	1499.559	978.128	990.719	282.875	1416.992	-38.955
2000	765.596	1538.676	1005.185	1066.982	285.288	1476.628	-38.565
2100	770.950	1576.162	1031.488	1143.814	287.619	1536.135	-38.208
2200	775.702	1612.138	1057.069	1221.152	289.863	1595.536	-37.882
2300	779.934	1646.714	1081.959	1298.937	292.012	1654.834	-37.582
2400	783.719	1679.990	1106.188	1377.124	294.011	1714.008	-37.304
2500	787.113	1712.053	1129.785	1455.668	295.865	1773.186	-37.048
2600	790.168	1742.984	1152.779	1534.535	297.546	1832.206	-36.809
2700	792.927	1772.858	1175.194	1613.692	299.055	1891.215	-36.587
2800	795.424	1801.741	1197.058	1693.112	300.372	1950.194	-36.381
2900	797.692	1829.694	1218.394	1772.769	301.471	2009.085	-36.187
3000	799.757	1856.772	1239.224	1852.643	302.386	2067.962	-36.006
3100	801.643	1883.027	1259.571	1932.715	303.058	2126.757	-35.835
3200	803.368	1908.506	1279.454	2012.966	303.516	2185.587	-35.675
3300	804.950	1933.251	1298.893	2093.383	303.745	2244.434	-35.526
3400	806.404	1957.303	1317.906	2173.952	303.725	2303.217	-35.384
3500	807.744	1980.699	1336.510	2254.660	303.459	2361.989	-35.250
3600	808.981	2003.471	1354.722	2335.498	302.961	2420.833	-35.125
3700	810.125	2025.652	1372.557	2416.454	302.209	2479.714	-35.007
3800	811.185	2047.271	1390.029	2497.520	301.180	2538.567	-34.894
3900	812.169	2068.355	1407.153	2578.688	299.907	2597.418	-34.788
4000	813.083	2088.929	1423.941	2659.951	298.376	2656.405	-34.688
4100	813.935	2109.016	1440.406	2741.303	296.561	2715.378	-34.594
4200	814.730	2128.640	1456.560	2822.736	294.481	2774.393	-34.504
4300	815.473	2147.820	1472.414	2904.247	292.126	2833.393	-34.418
4400	816.167	2166.575	1487.978	2985.829	289.503	2892.521	-34.338
4500	816.818	2184.924	1503.262	3067.479	286.622	2951.755	-34.262
4600	817.428	2202.884	1518.277	3149.191	283.445	3011.058	-34.191
4700	818.002	2220.470	1533.031	3230.963	279.980	3070.349	-34.122
4800	818.541	2237.697	1547.532	3312.791	276.267	3129.795	-34.058
4900	819.048	2254.580	1561.790	3394.670	272.247	3189.221	-33.997
5000	819.527	2271.132	1575.812	3476.599	267.991	3248.876	-33.940

3.80. 9,10[1',2']-Benzenoanthracene, 9,10-dihydro



Other names: Tribenzobicyclo[2.2.2]octatriene

Triptycene

Formula: C₂₀H₁₄

Mass: 254.325 g/mol

CAS Number: 477-75-8

Point Group: D_{3h}

Length: 10.60 Å

Width: 9.770 Å

Breadth: 7.410 Å

L/B Ratio: 1.085

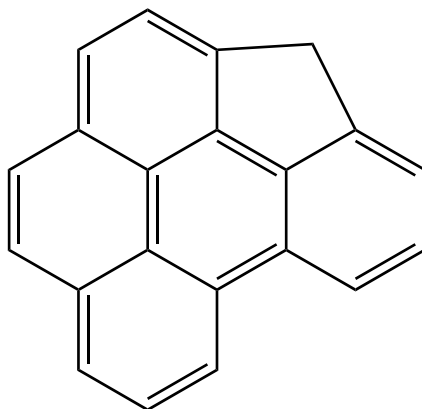
Cartesian coordinates:

C	0.5261	-1.2861	0.7047	C	0.8504	1.0985	0.7052	H	1.7918	-4.3799	-1.2399
C	0.5258	-1.2857	-0.7053	C	-0.0002	-0.0004	1.3084	H	1.5807	2.0423	-2.5018
C	0.9786	-2.3892	1.4069	C	-1.3770	0.1879	-0.7049	H	2.8987	3.7407	1.2397
C	0.9768	-2.3892	-1.4079	C	-1.3770	0.1869	0.7051	H	-0.0007	-0.0004	-2.4189
C	1.4336	-3.5008	0.6935	C	-2.5582	0.3499	-1.4072	H	1.5816	2.0408	2.5025
C	1.4325	-3.5008	-0.6951	C	-2.5585	0.3462	1.4076	H	0.0002	0.0005	2.4189
C	2.3163	2.9910	-0.6938	C	-3.7486	0.5107	-0.6939	H	-2.5589	0.3513	-2.5019
C	1.5803	2.0417	-1.4071	C	-3.7488	0.5088	0.6946	H	-2.5591	0.3448	2.5024
C	2.3165	2.9904	0.6948	H	2.8981	3.7420	-1.2382	H	-4.6895	0.6404	-1.2386
C	0.8504	1.0990	-0.7048	H	0.9799	-2.3896	2.5017	H	-4.6902	0.6346	1.2393
C	-0.0002	0.0006	-1.3085	H	0.9763	-2.3898	-2.5027				
C	1.5809	2.0407	1.4077	H	1.7946	-4.3795	1.2379				

Table 3.80: Table of thermodynamic data as a function of temperature for 9,10[1',2']-Benzenoanthracene, 9,10-dihydro.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-38.401	341.440	341.440	∞
100	84.990	301.398	629.832	-32.843	366.692	408.965	-213.617
200	163.142	382.604	486.021	-20.683	353.474	456.458	-119.212
250	211.345	424.118	469.464	-11.337	347.129	482.940	-100.903
298.15	259.565	465.463	465.463	0.000	341.440	509.625	-89.282
300	261.411	467.074	465.468	0.482	341.231	510.668	-88.913
350	310.163	511.065	468.831	14.782	335.968	539.335	-80.490
400	355.586	555.490	476.885	31.442	331.389	568.701	-74.263
450	396.776	599.794	488.084	50.269	327.429	598.607	-69.483
500	433.583	643.541	501.448	71.046	324.012	628.941	-65.704
600	495.285	728.270	532.249	117.612	318.515	690.472	-60.110
700	544.156	808.430	566.035	169.676	314.553	752.803	-56.174
800	583.498	883.751	601.092	226.127	311.913	815.597	-53.252
900	615.715	954.398	636.466	286.139	310.407	878.648	-50.994
1000	642.460	1020.697	671.608	349.088	309.868	941.823	-49.195
1100	664.897	1083.012	706.205	414.488	310.115	1005.019	-47.723
1200	683.870	1141.702	740.075	481.952	311.013	1068.151	-46.494
1300	700.021	1197.096	773.120	551.168	312.402	1131.194	-45.451
1400	713.849	1249.492	805.292	621.879	314.165	1194.120	-44.552
1500	725.751	1299.158	836.576	693.874	316.223	1256.909	-43.769
1600	736.046	1346.334	866.974	766.976	318.468	1319.547	-43.078
1700	744.993	1391.231	896.503	841.038	320.833	1382.022	-42.463
1800	752.806	1434.040	925.186	915.937	323.253	1444.406	-41.915
1900	759.657	1474.929	953.052	991.567	325.700	1506.614	-41.419
2000	765.691	1514.051	980.131	1067.841	328.123	1568.713	-40.970
2100	771.027	1551.541	1006.454	1144.682	330.463	1630.682	-40.560
2200	775.763	1587.521	1032.054	1222.026	332.714	1692.546	-40.185
2300	779.984	1622.100	1056.962	1299.817	334.868	1754.305	-39.841
2400	783.758	1655.377	1081.207	1378.008	336.872	1815.940	-39.522
2500	787.145	1687.441	1104.819	1456.556	338.730	1877.580	-39.229
2600	790.194	1718.374	1127.826	1535.426	340.413	1939.060	-38.955
2700	792.946	1748.249	1150.254	1614.585	341.925	2000.531	-38.702
2800	795.440	1777.132	1172.130	1694.006	343.243	2061.970	-38.466
2900	797.704	1805.085	1193.476	1773.665	344.344	2123.323	-38.244
3000	799.766	1832.164	1214.317	1853.540	345.260	2184.660	-38.038
3100	801.649	1858.419	1234.673	1933.613	345.932	2245.916	-37.843
3200	803.372	1883.898	1254.565	2013.865	346.391	2307.206	-37.661
3300	804.952	1908.644	1274.013	2094.282	346.620	2368.514	-37.490
3400	806.405	1932.696	1293.034	2174.851	346.601	2429.758	-37.328
3500	807.744	1956.091	1311.645	2255.559	346.334	2490.990	-37.175
3600	808.980	1978.863	1329.864	2336.396	345.836	2552.296	-37.032
3700	810.123	2001.044	1347.706	2417.352	345.084	2613.637	-36.897
3800	811.182	2022.663	1365.185	2498.418	344.055	2674.951	-36.769
3900	812.165	2043.747	1382.315	2579.586	342.782	2736.263	-36.647
4000	813.080	2064.321	1399.109	2660.849	341.251	2797.711	-36.534
4100	813.931	2084.409	1415.579	2742.200	339.435	2859.145	-36.425
4200	814.726	2104.032	1431.738	2823.633	337.355	2920.620	-36.322
4300	815.468	2123.212	1447.597	2905.143	334.999	2982.081	-36.224
4400	816.162	2141.967	1463.166	2986.725	332.376	3043.670	-36.132
4500	816.813	2160.316	1478.455	3068.374	329.494	3105.365	-36.045
4600	817.423	2178.275	1493.474	3150.087	326.316	3167.128	-35.963
4700	817.997	2195.861	1508.232	3231.858	322.852	3228.880	-35.884
4800	818.536	2213.088	1522.737	3313.685	319.137	3290.787	-35.810
4900	819.043	2229.971	1536.999	3395.564	315.117	3352.674	-35.739
5000	819.522	2246.523	1551.025	3477.493	310.860	3414.790	-35.673

3.81. 1*H*-Indeno[2,1,7-*cde*]pyrene



Other names: 3*H*-Indeno[2,1,7-*cde*]pyrene

Formula: C₂₁H₁₂

Mass: 264.320 g/mol

CAS Number: 59004-71-6

Point Group: C₁

Length: 11.70 Å

Width: 10.40 Å

Breadth: 4.595 Å

L/B Ratio: 1.124

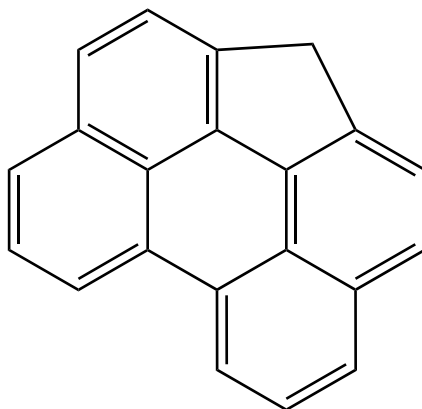
Cartesian coordinates:

C	3.2976	1.8480	0.0122	C	-0.2035	-1.5974	-0.0453	H	1.9424	2.7738	0.3350
C	2.9551	0.5537	0.0203	C	-0.6083	-2.9173	-0.0631	H	5.0048	-0.1924	0.1630
C	3.9531	-0.4936	0.1110	C	-1.9768	-3.2506	-0.0639	H	4.3283	-2.5883	0.1922
C	3.5809	-1.7904	0.1297	C	-2.9349	-2.2699	-0.0292	H	1.9325	-3.2374	0.0849
C	2.1970	-2.1688	0.0680	C	-0.8095	0.8079	-0.0358	H	-2.1396	3.9378	0.3478
C	1.5502	0.1772	-0.0462	C	-1.1882	-0.5660	-0.0336	H	0.2343	4.5960	0.0885
C	1.2115	-1.2336	-0.0084	C	-2.5567	-0.9030	-0.0037	H	0.1546	-3.7111	-0.0675
C	0.5914	1.1486	-0.1243	C	-3.5275	0.1349	0.0621	H	-2.2654	-4.3067	-0.0857
C	-1.3609	3.1908	0.1548	C	-3.1456	1.4477	0.1121	H	-4.0002	-2.5266	-0.0186
C	-0.0752	3.5479	0.0127	C	-1.7730	1.8023	0.0680	H	-4.5887	-0.1385	0.0825
C	0.9878	2.5666	-0.2945	H	1.3357	2.7329	-1.3405	H	-3.8953	2.2440	0.1843

Table 3.81: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[2,1,7-*cde*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-39.914	329.793	329.793	∞
100	86.980	316.140	660.240	-34.410	349.001	379.823	-198.395
200	172.481	401.352	509.492	-21.628	338.774	414.742	-108.317
250	221.217	445.045	492.214	-11.792	334.017	434.285	-90.737
298.15	268.451	488.060	488.060	0.000	329.793	453.990	-79.536
300	270.240	489.726	488.065	0.498	329.637	454.759	-79.179
350	317.232	534.950	491.529	15.197	325.751	475.930	-71.027
400	360.723	580.193	499.787	32.163	322.382	497.612	-64.980
450	400.064	624.994	511.216	51.200	319.466	519.695	-60.323
500	435.193	668.999	524.801	72.099	316.934	542.097	-56.631
600	494.036	753.759	555.963	118.678	312.801	587.539	-51.149
700	540.529	833.544	589.980	170.495	309.757	633.588	-47.278
800	577.798	908.242	625.146	226.477	307.681	679.994	-44.398
900	608.159	978.109	660.526	285.825	306.449	726.604	-42.170
1000	633.229	1043.523	695.590	347.933	305.950	773.320	-40.393
1100	654.156	1104.887	730.039	412.333	306.042	820.065	-38.941
1200	671.774	1162.583	763.704	478.654	306.625	866.764	-37.728
1300	686.715	1216.960	796.499	546.599	307.564	913.409	-36.700
1400	699.466	1268.329	828.384	615.924	308.766	959.974	-35.816
1500	710.410	1316.970	859.349	686.432	310.171	1006.447	-35.047
1600	719.855	1363.128	889.405	757.956	311.685	1052.815	-34.370
1700	728.048	1407.020	918.573	830.361	313.254	1099.068	-33.770
1800	735.189	1448.841	946.880	903.531	314.822	1145.277	-33.234
1900	741.443	1488.762	974.357	977.369	316.370	1191.359	-32.752
2000	746.943	1526.936	1001.039	1051.794	317.856	1237.382	-32.316
2100	751.802	1563.499	1026.958	1126.737	319.223	1283.322	-31.920
2200	756.111	1598.575	1052.149	1202.136	320.472	1329.201	-31.559
2300	759.948	1632.271	1076.644	1277.943	321.600	1375.026	-31.227
2400	763.376	1664.688	1100.475	1354.112	322.553	1420.768	-30.922
2500	766.450	1695.914	1123.672	1430.606	323.342	1466.561	-30.641
2600	769.216	1726.030	1146.264	1507.392	323.940	1512.236	-30.381
2700	771.712	1755.108	1168.278	1584.441	324.350	1557.948	-30.140
2800	773.972	1783.215	1189.741	1661.727	324.554	1603.665	-29.916
2900	776.024	1810.411	1210.677	1739.228	324.530	1649.337	-29.707
3000	777.891	1836.751	1231.109	1816.925	324.311	1695.034	-29.513
3100	779.596	1862.286	1251.060	1894.801	323.838	1740.683	-29.330
3200	781.155	1887.062	1270.550	1972.840	323.145	1786.408	-29.160
3300	782.585	1911.122	1289.599	2051.028	322.217	1832.188	-29.001
3400	783.899	1934.504	1308.224	2129.353	321.033	1877.933	-28.850
3500	785.110	1957.245	1326.444	2207.804	319.598	1923.702	-28.709
3600	786.227	1979.378	1344.275	2286.372	317.927	1969.584	-28.577
3700	787.261	2000.935	1361.733	2365.047	315.998	2015.528	-28.454
3800	788.218	2021.942	1378.831	2443.821	313.791	2061.482	-28.336
3900	789.107	2042.428	1395.585	2522.688	311.337	2107.457	-28.226
4000	789.933	2062.417	1412.007	2601.641	308.623	2153.606	-28.123
4100	790.702	2081.932	1428.110	2680.673	305.623	2199.768	-28.025
4200	791.420	2100.995	1443.905	2759.779	302.359	2246.001	-27.933
4300	792.090	2119.626	1459.403	2838.955	298.819	2292.245	-27.845
4400	792.718	2137.843	1474.616	2918.196	295.011	2338.645	-27.763
4500	793.305	2155.664	1489.553	2997.497	290.945	2385.178	-27.686
4600	793.856	2173.106	1504.224	3076.856	286.582	2431.811	-27.614
4700	794.374	2190.184	1518.638	3156.268	281.934	2478.454	-27.544
4800	794.860	2206.914	1532.803	3235.730	277.036	2525.280	-27.480
4900	795.319	2223.308	1546.729	3315.239	271.831	2572.107	-27.418
5000	795.751	2239.380	1560.422	3394.792	266.392	2619.187	-27.362

3.82. 1*H*-Cyclopenta[ghi]perylene



Formula: C₂₁H₁₂
Mass: 264.320 g/mol
CAS Number: 83899-23-4
Point Group: C_{2v}

Length: 11.77 Å
Width: 9.947 Å
Breadth: 4.180 Å
L/B Ratio: 1.183

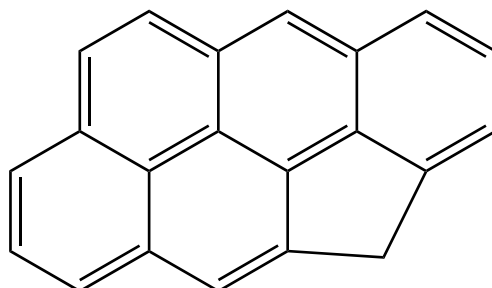
Cartesian coordinates:

C	0.2765	3.1644	0.0004	C	-0.8672	-1.4340	-0.0023	H	0.3341	3.8114	0.8929
C	1.3908	2.1202	-0.0022	C	-1.7504	-2.4908	0.0000	H	3.3525	3.0650	0.0054
C	2.7996	2.1208	0.0022	C	-3.1494	-2.2582	0.0020	H	4.5705	0.9100	0.0067
C	3.4742	0.9108	0.0033	C	-3.6915	-0.9968	0.0026	H	-4.3433	1.6889	0.0059
C	0.7912	0.8738	-0.0054	C	1.4101	-0.3765	-0.0030	H	-2.7698	3.6002	0.0047
C	-1.0020	2.3292	-0.0022	C	2.8162	-0.3566	0.0009	H	-1.3819	-3.5239	0.0007
C	-0.6275	0.9977	-0.0054	C	3.4626	-1.6220	0.0030	H	-3.8129	-3.1302	0.0034
C	-3.2636	1.4997	0.0028	C	2.7099	-2.7703	0.0022	H	-4.7767	-0.8495	0.0047
C	-2.3892	2.5744	0.0021	C	1.2918	-2.7567	-0.0000	H	4.5569	-1.6652	0.0052
C	-2.8353	0.1373	0.0005	C	0.6053	-1.5626	-0.0023	H	3.2120	-3.7442	0.0034
C	-1.4540	-0.1262	-0.0032	H	0.3327	3.8177	-0.8879	H	0.7497	-3.7102	0.0004

Table 3.82: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*ghi*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} [°]	<i>S</i> [°]	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> [°] (<i>T</i>) - <i>H</i> [°] (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> [°]	Δ _{<i>f</i>} <i>G</i> [°]	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-37.584	371.497	371.497	∞
100	78.617	301.860	627.287	-32.543	392.574	424.823	-221.900
200	162.832	380.755	484.151	-20.679	381.427	461.515	-120.533
250	211.507	422.282	467.598	-11.329	376.185	482.143	-100.736
298.15	258.953	463.601	463.601	0.000	371.497	502.987	-88.119
300	260.755	465.209	463.606	0.481	371.324	503.802	-87.718
350	308.181	509.001	466.956	14.716	366.974	526.235	-78.535
400	352.234	553.072	474.966	31.242	363.166	549.245	-71.723
450	392.199	596.908	486.084	49.871	359.841	572.708	-66.477
500	427.963	640.117	499.334	70.392	356.932	596.535	-62.318
600	488.013	723.668	529.820	116.309	352.138	644.929	-56.145
700	535.550	802.605	563.208	167.578	348.545	694.033	-51.788
800	573.680	876.697	597.814	223.107	346.015	743.565	-48.549
900	604.736	946.120	632.699	282.079	344.408	793.352	-46.044
1000	630.364	1011.204	667.330	343.873	343.596	843.285	-44.048
1100	651.738	1072.316	701.398	408.010	343.424	893.275	-42.417
1200	669.716	1129.818	734.728	474.108	343.783	943.241	-41.057
1300	684.948	1184.041	767.225	541.862	344.532	993.170	-39.905
1400	697.936	1235.289	798.844	611.023	345.569	1043.033	-38.915
1500	709.076	1283.832	829.573	681.388	346.832	1092.815	-38.054
1600	718.682	1329.908	859.416	752.787	348.220	1142.501	-37.298
1700	727.010	1373.734	888.392	825.081	349.679	1192.080	-36.627
1800	734.265	1415.499	916.525	898.153	351.150	1241.621	-36.030
1900	740.615	1455.372	943.844	971.904	352.610	1291.040	-35.492
2000	746.198	1493.506	970.380	1046.251	354.017	1340.403	-35.007
2100	751.128	1530.035	996.167	1121.122	355.313	1389.688	-34.566
2200	755.498	1565.080	1021.236	1196.458	356.498	1438.915	-34.163
2300	759.389	1598.751	1045.618	1272.206	357.567	1488.091	-33.795
2400	762.864	1631.145	1069.344	1348.322	358.467	1537.186	-33.455
2500	765.979	1662.351	1092.444	1424.767	359.207	1586.335	-33.144
2600	768.782	1692.449	1114.946	1501.507	359.759	1635.367	-32.854
2700	771.310	1721.511	1136.876	1578.514	360.128	1684.438	-32.587
2800	773.599	1749.604	1158.260	1655.761	360.293	1733.515	-32.338
2900	775.676	1776.787	1179.123	1733.227	360.233	1782.549	-32.107
3000	777.567	1803.116	1199.486	1810.890	359.981	1831.609	-31.890
3100	779.293	1828.641	1219.372	1888.735	359.477	1880.622	-31.688
3200	780.871	1853.408	1238.800	1966.744	358.754	1929.711	-31.499
3300	782.319	1877.459	1257.791	2044.904	357.799	1978.858	-31.322
3400	783.649	1900.834	1276.362	2123.204	356.589	2027.969	-31.155
3500	784.874	1923.568	1294.530	2201.631	355.129	2077.106	-30.998
3600	786.004	1945.694	1312.312	2280.175	353.436	2126.356	-30.852
3700	787.050	1967.244	1329.723	2358.829	351.485	2175.669	-30.714
3800	788.019	1988.247	1346.777	2437.583	349.257	2224.992	-30.584
3900	788.917	2008.728	1363.489	2516.430	346.783	2274.337	-30.461
4000	789.753	2028.712	1379.871	2595.364	344.051	2323.856	-30.346
4100	790.531	2048.223	1395.935	2674.379	341.034	2373.389	-30.237
4200	791.257	2067.281	1411.693	2753.469	337.753	2422.993	-30.134
4300	791.935	2085.908	1427.157	2832.629	334.197	2472.608	-30.036
4400	792.569	2104.122	1442.336	2911.854	330.373	2522.381	-29.944
4500	793.163	2121.940	1457.242	2991.141	326.293	2572.286	-29.858
4600	793.721	2139.379	1471.882	3070.486	321.917	2622.291	-29.776
4700	794.244	2156.454	1486.266	3149.884	317.255	2672.307	-29.699
4800	794.736	2173.181	1500.403	3229.333	312.345	2722.507	-29.626
4900	795.199	2189.573	1514.301	3308.831	307.128	2772.707	-29.557
5000	795.636	2205.642	1527.968	3388.373	301.677	2823.160	-29.493

3.83. 4*H*-Benzo[*def*]cyclopenta[*mno*]chrysene



Formula: C₂₁H₁₂
Mass: 264.320 g/mol
CAS Number: 59004-72-7
Point Group: C_s

Length: 13.52 Å
Width: 9.654 Å
Breadth: 4.178 Å
L/B Ratio: 1.401

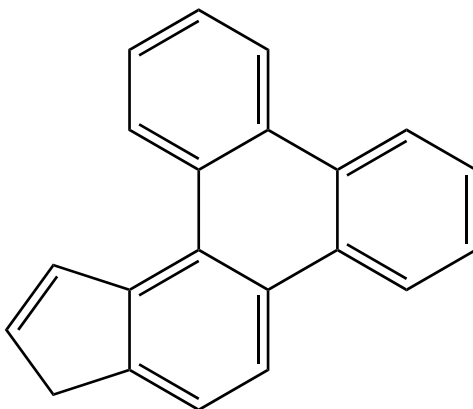
Cartesian coordinates:

C	-1.8548	2.4402	0.0000	C	-2.7517	1.2060	0.0000	H	-2.0391	3.0681	0.8896
C	-0.4368	1.8806	0.0000	C	-4.0977	0.9659	-0.0000	H	1.0331	3.4558	0.0000
C	0.8279	2.3806	0.0000	C	-4.5403	-0.3915	-0.0000	H	4.9890	-1.0422	-0.0000
C	1.9542	1.4619	-0.0000	C	-3.6963	-1.4798	-0.0000	H	5.3659	1.4048	-0.0000
C	4.1322	-0.3598	-0.0000	C	2.8359	-0.8636	0.0000	H	3.4798	2.9993	-0.0000
C	4.3388	1.0234	-0.0000	C	1.7649	0.0567	-0.0000	H	-1.4884	-3.3120	-0.0000
C	3.2826	1.9213	-0.0000	C	0.4433	-0.4678	0.0000	H	-4.8344	1.7743	-0.0000
C	-0.5693	0.4556	0.0000	C	0.1041	-1.8570	0.0000	H	-5.6227	-0.5637	-0.0000
C	-1.2290	-2.2476	0.0000	C	1.2454	-2.7514	0.0000	H	-4.0963	-2.4988	-0.0000
C	-2.2854	-1.2827	-0.0000	C	2.5154	-2.2799	0.0000	H	1.0476	-3.8291	0.0000
C	-1.9128	0.0587	0.0000	H	-2.0391	3.0681	-0.8896	H	3.3622	-2.9765	0.0000

Table 3.83: Table of thermodynamic data as a function of temperature for 4*H*-Benzo[*def*]cyclopenta[*mno*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-37.529	356.018	356.018	∞
100	78.176	308.004	633.010	-32.501	377.137	408.772	-213.516
200	162.611	386.632	490.004	-20.674	365.953	444.865	-116.185
250	211.473	428.131	473.452	-11.330	360.705	465.201	-97.196
298.15	259.027	469.455	469.455	0.000	356.018	485.763	-85.102
300	260.831	471.062	469.460	0.481	355.845	486.567	-84.717
350	308.294	514.870	472.811	14.721	351.500	508.707	-75.919
400	352.342	558.956	480.824	31.253	347.698	531.423	-69.395
450	392.284	602.804	491.945	49.886	344.378	554.592	-64.374
500	428.022	646.021	505.199	70.411	341.472	578.124	-60.395
600	488.032	729.579	535.692	116.332	336.682	625.927	-54.491
700	535.549	808.516	569.086	167.601	333.090	674.440	-50.326
800	573.674	882.608	603.695	223.130	330.559	723.380	-47.231
900	604.731	952.030	638.584	282.101	328.952	772.577	-44.838
1000	630.364	1017.113	673.218	343.896	328.139	821.919	-42.932
1100	651.743	1078.226	707.287	408.033	327.968	871.317	-41.375
1200	669.725	1135.728	740.619	474.131	328.328	920.693	-40.076
1300	684.961	1189.953	773.117	541.886	329.078	970.031	-38.976
1400	697.951	1241.202	804.738	611.049	330.116	1019.303	-38.030
1500	709.093	1289.745	835.469	681.415	331.380	1068.494	-37.207
1600	718.700	1335.823	865.313	752.816	332.771	1117.588	-36.485
1700	727.029	1379.650	894.290	825.113	334.231	1166.575	-35.844
1800	734.284	1421.416	922.423	898.186	335.704	1215.524	-35.273
1900	740.634	1461.290	949.743	971.939	337.165	1264.352	-34.759
2000	746.216	1499.425	976.281	1046.287	338.575	1313.123	-34.295
2100	751.145	1535.955	1002.069	1121.161	339.873	1361.816	-33.873
2200	755.516	1571.001	1027.138	1196.498	341.059	1410.451	-33.488
2300	759.405	1604.672	1051.521	1272.248	342.130	1459.035	-33.135
2400	762.880	1637.067	1075.248	1348.365	343.031	1507.538	-32.810
2500	765.995	1668.274	1098.349	1424.812	343.773	1556.094	-32.512
2600	768.796	1698.372	1120.851	1501.554	344.327	1604.534	-32.235
2700	771.324	1727.435	1142.782	1578.562	344.697	1653.013	-31.979
2800	773.612	1755.528	1164.167	1655.811	344.864	1701.497	-31.741
2900	775.689	1782.712	1185.030	1733.277	344.805	1749.939	-31.519
3000	777.580	1809.041	1205.394	1810.942	344.554	1798.406	-31.312
3100	779.304	1834.567	1225.280	1888.788	344.051	1846.827	-31.118
3200	780.882	1859.334	1244.709	1966.798	343.330	1895.324	-30.937
3300	782.329	1883.385	1263.701	2044.960	342.375	1943.877	-30.768
3400	783.659	1906.760	1282.272	2123.260	341.166	1992.396	-30.609
3500	784.884	1929.494	1300.441	2201.688	339.707	2040.940	-30.459
3600	786.014	1951.621	1318.223	2280.234	338.015	2089.597	-30.319
3700	787.059	1973.172	1335.634	2358.888	336.065	2138.318	-30.187
3800	788.027	1994.174	1352.689	2437.643	333.838	2187.048	-30.062
3900	788.926	2014.655	1369.401	2516.491	331.366	2235.800	-29.945
4000	789.761	2034.640	1385.783	2595.426	328.634	2284.727	-29.835
4100	790.539	2054.151	1401.848	2674.441	325.618	2333.667	-29.731
4200	791.265	2073.210	1417.607	2753.532	322.337	2382.678	-29.632
4300	791.942	2091.837	1433.071	2832.693	318.782	2431.701	-29.539
4400	792.576	2110.050	1448.251	2911.919	314.959	2480.880	-29.451
4500	793.170	2127.869	1463.156	2991.207	310.880	2530.192	-29.369
4600	793.727	2145.308	1477.796	3070.552	306.504	2579.605	-29.292
4700	794.250	2162.383	1492.181	3149.951	301.843	2629.028	-29.218
4800	794.742	2179.110	1506.318	3229.401	296.933	2678.634	-29.149
4900	795.205	2195.502	1520.217	3308.898	291.717	2728.241	-29.083
5000	795.642	2211.572	1533.884	3388.441	286.266	2778.102	-29.022

3.84. 1*H*-Cyclopenta[*a*]triphenylene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 196-87-2
Point Group: C₁

Length: 13.04 Å
Width: 10.48 Å
Breadth: 4.470 Å
L/B Ratio: 1.244

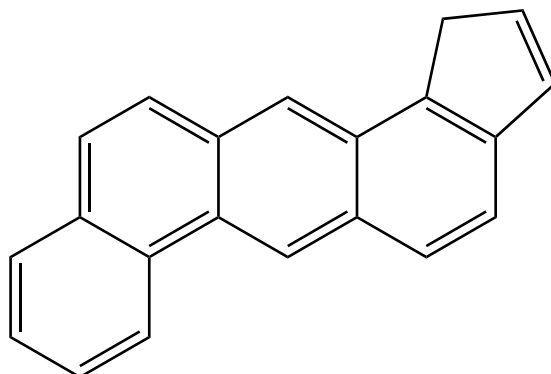
Cartesian coordinates:

C	4.4205	-0.4701	-0.3606	C	-1.5440	-3.6246	0.0631	H	2.9477	-2.0706	-0.5121
C	4.3483	1.0067	-0.1019	C	-0.1653	-3.6844	0.2743	H	2.7629	3.3754	0.3522
C	3.1883	-1.0204	-0.3351	C	0.5835	-2.5237	0.2890	H	0.2757	3.3563	0.3788
C	2.1817	0.0137	-0.0596	C	-2.0865	0.0797	-0.0927	H	-3.2445	-2.3358	-0.2185
C	2.8749	1.2364	0.0504	C	-1.3481	1.2627	0.0642	H	-2.1356	-4.5448	0.0292
C	2.2100	2.4374	0.2447	C	-2.0345	2.4917	0.0946	H	0.3207	-4.6530	0.4305
C	0.8275	2.4105	0.2697	C	-3.4060	2.5471	-0.0499	H	1.6609	-2.6025	0.4838
C	0.7794	-0.0327	0.0557	C	-4.1363	1.3693	-0.2327	H	-1.4639	3.4224	0.2314
C	0.1059	1.2089	0.1468	C	-3.4829	0.1540	-0.2511	H	-3.9238	3.5114	-0.0257
C	-0.0053	-1.2624	0.0841	H	5.3643	-0.9800	-0.5440	H	-5.2230	1.4140	-0.3569
C	-1.4063	-1.2043	-0.0479	H	4.9068	1.2929	0.8082	H	-4.0541	-0.7771	-0.3850
C	-2.1539	-2.3954	-0.0824	H	4.7730	1.5892	-0.9400				

Table 3.84: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*a*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.404	386.650	386.650	∞
100	92.603	327.074	681.495	-35.442	410.295	450.096	-235.101
200	176.980	415.756	526.592	-22.167	397.866	494.836	-129.235
250	226.581	460.524	508.883	-12.090	391.955	519.763	-108.596
298.15	275.559	504.623	504.623	0.000	386.650	544.871	-95.457
300	277.427	506.333	504.628	0.512	386.454	545.852	-95.039
350	326.711	552.834	508.188	15.626	381.535	572.818	-85.487
400	372.609	599.501	516.686	33.126	377.244	600.437	-78.407
450	414.278	645.836	528.467	52.816	373.519	628.564	-72.960
500	451.576	691.453	542.492	74.480	370.291	657.095	-68.645
600	514.235	779.548	574.725	122.894	365.064	714.974	-62.243
700	563.955	862.695	609.986	176.897	361.267	773.617	-57.727
800	604.011	940.708	646.503	235.364	358.723	832.702	-54.369
900	636.815	1013.806	683.297	297.458	357.264	892.037	-51.771
1000	664.044	1082.353	719.812	362.542	356.737	951.492	-49.700
1100	686.882	1146.746	755.727	430.121	356.969	1010.970	-48.006
1200	706.191	1207.363	790.863	499.801	357.832	1070.383	-46.592
1300	722.626	1264.555	825.122	571.263	359.168	1129.713	-45.392
1400	736.696	1318.635	858.459	644.247	360.864	1188.930	-44.359
1500	748.806	1369.885	890.861	718.537	362.844	1248.016	-43.459
1600	759.281	1418.554	922.333	793.954	364.999	1306.956	-42.667
1700	768.385	1464.865	952.896	870.348	367.263	1365.739	-41.963
1800	776.334	1509.015	982.575	947.592	369.572	1424.437	-41.335
1900	783.306	1551.180	1011.400	1025.582	371.899	1482.966	-40.769
2000	789.446	1591.518	1039.405	1104.226	374.194	1541.393	-40.256
2100	794.876	1630.169	1066.623	1183.447	376.394	1599.695	-39.789
2200	799.697	1667.260	1093.087	1263.181	378.498	1657.899	-39.363
2300	803.992	1702.904	1118.831	1343.369	380.496	1716.006	-38.971
2400	807.834	1737.205	1143.886	1423.964	382.334	1773.994	-38.609
2500	811.281	1770.253	1168.284	1504.923	384.018	1831.997	-38.277
2600	814.384	1802.134	1192.053	1586.209	385.518	1889.844	-37.967
2700	817.186	1832.922	1215.222	1667.790	386.837	1947.692	-37.680
2800	819.724	1862.688	1237.818	1749.637	387.953	2005.516	-37.413
2900	822.029	1891.494	1259.864	1831.727	388.843	2063.259	-37.163
3000	824.129	1919.398	1281.386	1914.036	389.539	2120.995	-36.929
3100	826.045	1946.453	1302.406	1996.546	389.981	2178.654	-36.709
3200	827.799	1972.707	1322.944	2079.240	390.201	2236.358	-36.504
3300	829.408	1998.205	1343.022	2162.101	390.182	2294.089	-36.312
3400	830.888	2022.987	1362.659	2245.117	389.905	2351.759	-36.130
3500	832.251	2047.093	1381.871	2328.275	389.371	2409.426	-35.958
3600	833.509	2070.556	1400.677	2411.564	388.597	2467.177	-35.797
3700	834.673	2093.409	1419.092	2494.974	387.559	2524.971	-35.645
3800	835.752	2115.683	1437.131	2578.496	386.234	2582.745	-35.502
3900	836.753	2137.405	1454.810	2662.122	384.656	2640.521	-35.365
4000	837.684	2158.602	1472.141	2745.844	382.810	2698.448	-35.237
4100	838.551	2179.297	1489.137	2829.656	380.669	2756.365	-35.116
4200	839.360	2199.514	1505.811	2913.552	378.255	2814.332	-35.001
4300	840.116	2219.273	1522.174	2997.527	375.556	2872.289	-34.891
4400	840.823	2238.595	1538.238	3081.574	372.579	2930.385	-34.787
4500	841.486	2257.499	1554.012	3165.690	369.335	2988.598	-34.690
4600	842.107	2276.000	1569.507	3249.870	365.784	3046.887	-34.598
4700	842.691	2294.117	1584.732	3334.110	361.936	3105.170	-34.509
4800	843.240	2311.865	1599.697	3418.407	357.830	3163.619	-34.426
4900	843.757	2329.257	1614.409	3502.757	353.406	3222.052	-34.347
5000	844.244	2346.308	1628.877	3587.157	348.738	3280.728	-34.273

3.85. 1*H*-Benzo[*a*]cyclopent[*h*]anthracene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 240-44-8
Point Group: C_s

Length: 14.96 Å
Width: 8.709 Å
Breadth: 4.177 Å
L/B Ratio: 1.718

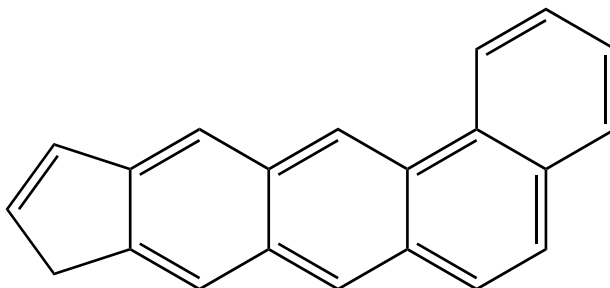
Cartesian coordinates:

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C	3.4263	-0.8175	-0.0000	C	-3.0471	-0.3936	0.0000	H	-4.0188	2.8918	-0.0000
C	4.8237	-0.6529	0.0000	C	-3.8725	0.7231	-0.0000	H	-1.1862	-2.3754	0.0000
C	5.3761	0.6119	0.0000	C	-3.3409	2.0327	-0.0000	H	0.7168	2.2481	-0.0000
C	4.5475	1.7412	0.0000	C	-1.9830	2.1871	-0.0000	H	1.0651	-3.3115	-0.0000
C	2.8455	-2.1381	-0.0000	C	-5.2659	0.2798	0.0000	H	3.5254	-2.9979	-0.0000
C	1.5071	-2.3084	-0.0000	C	-5.2934	-1.0721	0.0000	H	5.4689	-1.5388	-0.0000
C	0.6105	-1.1764	-0.0000	C	-3.8952	-1.6313	0.0000	H	6.4636	0.7384	0.0000
C	1.1488	0.1421	0.0000	H	-3.7064	-2.2606	-0.8893	H	4.9938	2.7409	0.0000
C	-0.7634	-1.3630	0.0000	H	-3.7064	-2.2606	0.8893	H	2.5124	2.4730	0.0000
C	-1.6352	-0.2599	0.0000	H	-6.1124	0.9642	-0.0000				

Table 3.85: Table of thermodynamic data as a function of temperature for 1*H*-Benzo[*a*]cyclopent[*h*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.475	371.086	371.086	∞
100	92.578	328.145	683.330	-35.518	394.655	434.349	-226.876
200	177.386	416.864	528.042	-22.236	382.234	478.982	-125.095
250	227.318	461.761	510.277	-12.129	376.352	503.851	-105.272
298.15	276.420	506.003	506.003	0.000	371.086	528.896	-92.659
300	278.290	507.719	506.008	0.513	370.893	529.875	-92.257
350	327.542	554.351	509.579	15.671	366.016	556.768	-83.091
400	373.336	601.123	518.100	33.209	361.764	584.309	-76.301
450	414.886	647.537	529.908	52.933	358.072	612.352	-71.079
500	452.079	693.212	543.962	74.625	354.872	640.797	-66.942
600	514.607	781.386	576.250	123.081	349.688	698.496	-60.808
700	564.286	864.586	611.559	177.119	345.926	756.951	-56.483
800	604.347	942.643	648.119	235.619	343.415	815.846	-53.268
900	637.174	1015.782	684.951	297.748	341.990	874.984	-50.782
1000	664.426	1084.369	721.500	362.869	341.500	934.240	-48.799
1100	687.280	1148.798	757.447	430.487	341.771	993.514	-47.177
1200	706.596	1209.450	792.611	500.207	342.674	1052.721	-45.823
1300	723.031	1266.675	826.898	571.710	344.051	1111.841	-44.673
1400	737.094	1320.785	860.261	644.734	345.787	1170.844	-43.684
1500	749.193	1372.062	892.687	719.063	347.807	1229.714	-42.822
1600	759.654	1420.756	924.182	794.518	350.000	1288.435	-42.062
1700	768.743	1467.089	954.766	870.948	352.300	1346.996	-41.387
1800	776.675	1511.258	984.465	948.228	354.645	1405.471	-40.785
1900	783.630	1553.441	1013.309	1026.251	357.004	1463.774	-40.241
2000	789.754	1593.795	1041.332	1104.926	359.331	1521.974	-39.749
2100	795.167	1632.461	1068.567	1184.178	361.561	1580.048	-39.301
2200	799.972	1669.565	1095.047	1263.940	363.693	1638.022	-38.891
2300	804.253	1705.222	1120.807	1344.155	365.718	1695.898	-38.514
2400	808.080	1739.533	1145.877	1424.775	367.582	1753.654	-38.166
2500	811.514	1772.591	1170.288	1505.758	369.289	1811.424	-37.847
2600	814.605	1804.481	1194.070	1587.066	370.812	1869.037	-37.549
2700	817.395	1835.277	1217.252	1668.669	372.152	1926.649	-37.273
2800	819.922	1865.050	1239.859	1750.537	373.289	1984.237	-37.016
2900	822.217	1893.863	1261.917	1832.645	374.198	2041.744	-36.775
3000	824.307	1921.773	1283.449	1914.973	374.913	2099.242	-36.550
3100	826.214	1948.834	1304.479	1997.501	375.372	2156.663	-36.339
3200	827.960	1975.093	1325.027	2080.211	375.608	2214.129	-36.141
3300	829.561	2000.596	1345.114	2163.088	375.605	2271.621	-35.956
3400	831.033	2025.383	1364.760	2246.119	375.343	2329.052	-35.781
3500	832.389	2049.492	1383.981	2329.291	374.823	2386.479	-35.616
3600	833.641	2072.959	1402.794	2412.593	374.062	2443.990	-35.461
3700	834.799	2095.816	1421.217	2496.016	373.037	2501.544	-35.315
3800	835.872	2118.093	1439.264	2579.550	371.724	2559.077	-35.176
3900	836.868	2139.818	1456.950	2663.188	370.158	2616.612	-35.045
4000	837.794	2161.018	1474.287	2746.921	368.324	2674.297	-34.922
4100	838.657	2181.716	1491.290	2830.744	366.194	2731.973	-34.805
4200	839.461	2201.935	1507.971	2914.651	363.790	2789.697	-34.694
4300	840.213	2221.697	1524.340	2998.635	361.100	2847.412	-34.588
4400	840.916	2241.021	1540.409	3082.692	358.133	2905.266	-34.489
4500	841.575	2259.926	1556.189	3166.817	354.898	2963.236	-34.396
4600	842.193	2278.430	1571.690	3251.005	351.356	3021.282	-34.307
4700	842.774	2296.549	1586.920	3335.254	347.517	3079.322	-34.222
4800	843.320	2314.298	1601.890	3419.559	343.418	3137.528	-34.143
4900	843.834	2331.692	1616.607	3503.917	339.002	3195.718	-34.066
5000	844.318	2348.745	1631.080	3588.325	334.342	3254.150	-33.995

3.86. 9*H*-Benzo[*a*]cyclopent[*i*]anthracene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 226-78-8
Point Group: C_s

Length: 15.61 Å
Width: 8.918 Å
Breadth: 4.175 Å
L/B Ratio: 1.751

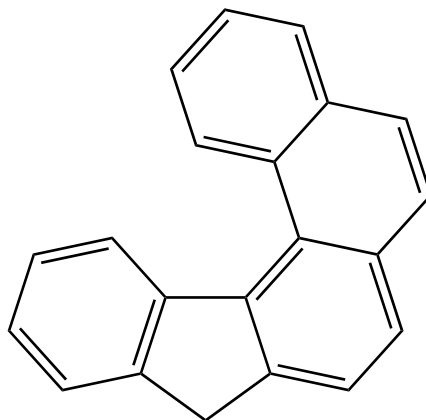
Cartesian coordinates:

C	5.8046	-0.7033	0.0000	C	-0.9569	1.4088	0.0000	H	4.8860	-2.6912	0.0000
C	5.2768	0.7074	-0.0000	C	-2.0562	2.3445	0.0000	H	2.9783	2.5001	-0.0000
C	4.8024	-1.6055	0.0000	C	-3.3362	1.9166	0.0000	H	2.0292	-2.4546	0.0000
C	3.5166	-0.9039	0.0000	C	-2.6096	-0.4382	0.0000	H	0.5649	2.9365	0.0000
C	3.7890	0.5119	-0.0000	C	-3.6482	0.5084	0.0000	H	-0.3896	-1.9678	0.0000
C	2.7827	1.4227	-0.0000	C	-4.9868	0.0736	0.0000	H	-1.8185	3.4146	0.0000
C	2.2427	-1.3806	0.0000	C	-5.2811	-1.2746	-0.0000	H	-4.1704	2.6276	0.0000
C	1.1612	-0.4421	0.0000	C	-4.2476	-2.2204	-0.0000	H	-5.7926	0.8164	0.0000
C	1.4288	0.9515	0.0000	C	-2.9311	-1.8084	0.0000	H	-6.3228	-1.6113	-0.0000
C	0.3563	1.8593	0.0000	H	6.8733	-0.9111	0.0000	H	-4.4901	-3.2880	-0.0000
C	-0.1714	-0.8875	0.0000	H	5.6194	1.2691	0.8884	H	-2.1085	-2.5399	-0.0000
C	-1.2280	0.0125	0.0000	H	5.6194	1.2691	-0.8884				

Table 3.86: Table of thermodynamic data as a function of temperature for 9*H*-Benzo[*a*]cyclopent[*i*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.137	366.625	366.625	∞
100	91.235	325.084	678.143	-35.306	390.406	430.405	-224.816
200	176.341	413.018	523.692	-22.135	377.873	475.391	-124.157
250	226.286	457.683	506.004	-12.080	371.939	500.457	-104.563
298.15	275.419	501.746	501.746	0.000	366.625	525.704	-92.099
300	277.290	503.456	501.751	0.511	366.429	526.690	-91.703
350	326.581	549.937	505.310	15.620	361.503	553.800	-82.648
400	372.415	596.582	513.805	33.111	357.204	581.565	-75.943
450	414.009	642.891	525.580	52.790	353.468	609.838	-70.787
500	451.250	688.476	539.598	74.439	350.225	638.517	-66.704
600	513.883	776.508	571.811	122.818	344.963	696.697	-60.652
700	563.668	859.605	607.050	176.788	341.134	755.646	-56.386
800	603.827	937.586	643.546	235.232	338.566	815.043	-53.216
900	636.739	1010.668	680.321	297.313	337.094	874.690	-50.765
1000	664.063	1079.213	716.819	362.394	336.564	934.460	-48.810
1100	686.975	1143.611	752.721	429.979	336.801	994.251	-47.212
1200	706.339	1204.239	787.846	499.671	337.677	1053.977	-45.877
1300	722.813	1261.444	822.098	571.150	339.030	1113.619	-44.745
1400	736.908	1315.539	855.429	644.154	340.746	1173.146	-43.770
1500	749.033	1366.804	887.827	718.466	342.748	1232.541	-42.920
1600	759.515	1415.489	919.297	793.906	344.926	1291.789	-42.172
1700	768.621	1461.814	949.858	870.324	347.213	1350.877	-41.507
1800	776.569	1505.977	979.537	947.592	349.547	1409.880	-40.913
1900	783.536	1548.154	1008.362	1025.605	351.896	1468.712	-40.377
2000	789.670	1588.504	1036.368	1104.271	354.214	1527.441	-39.892
2100	795.092	1627.166	1063.587	1183.515	356.437	1586.044	-39.450
2200	799.904	1664.267	1090.053	1263.269	358.561	1644.548	-39.046
2300	804.192	1699.920	1115.799	1343.478	360.580	1702.954	-38.674
2400	808.025	1734.229	1140.857	1424.093	362.437	1761.239	-38.332
2500	811.463	1767.285	1165.257	1505.070	364.140	1819.540	-38.016
2600	814.558	1799.172	1189.029	1586.374	365.658	1877.684	-37.722
2700	817.353	1829.967	1212.200	1667.972	366.993	1935.827	-37.450
2800	819.883	1859.739	1234.798	1749.836	368.126	1993.946	-37.197
2900	822.181	1888.551	1256.847	1831.941	369.031	2051.984	-36.959
3000	824.273	1916.460	1278.371	1914.265	369.743	2110.014	-36.738
3100	826.183	1943.519	1299.393	1996.789	370.199	2167.966	-36.529
3200	827.931	1969.777	1319.935	2079.496	370.432	2225.964	-36.334
3300	829.534	1995.279	1340.015	2162.370	370.426	2283.987	-36.152
3400	831.008	2020.065	1359.654	2245.399	370.161	2341.950	-35.979
3500	832.366	2044.174	1378.869	2328.568	369.639	2399.909	-35.816
3600	833.619	2067.640	1397.677	2411.868	368.876	2457.952	-35.663
3700	834.778	2090.496	1416.094	2495.289	367.848	2516.037	-35.519
3800	835.852	2112.773	1434.136	2578.821	366.534	2574.102	-35.383
3900	836.849	2134.498	1451.817	2662.457	364.965	2632.169	-35.253
4000	837.776	2155.697	1469.150	2746.188	363.129	2690.386	-35.132
4100	838.640	2176.394	1486.148	2830.010	360.997	2748.594	-35.017
4200	839.445	2196.613	1502.824	2913.914	358.592	2806.851	-34.908
4300	840.198	2216.375	1519.189	2997.897	355.901	2865.098	-34.803
4400	840.902	2235.699	1535.255	3081.952	352.932	2923.484	-34.705
4500	841.561	2254.604	1551.031	3166.076	349.696	2981.986	-34.613
4600	842.180	2273.107	1566.528	3250.263	346.152	3040.565	-34.526
4700	842.761	2291.225	1581.755	3334.511	342.311	3099.137	-34.442
4800	843.307	2308.974	1596.721	3418.814	338.212	3157.875	-34.364
4900	843.822	2326.368	1611.435	3503.171	333.795	3216.597	-34.289
5000	844.307	2343.420	1625.905	3587.578	329.133	3275.562	-34.219

3.87. 9*H*-Indeno[2,1-*c*]phenanthrene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 192-87-0
Point Group: C₁

Length: 12.36 Å
Width: 10.16 Å
Breadth: 5.339 Å
L/B Ratio: 1.216

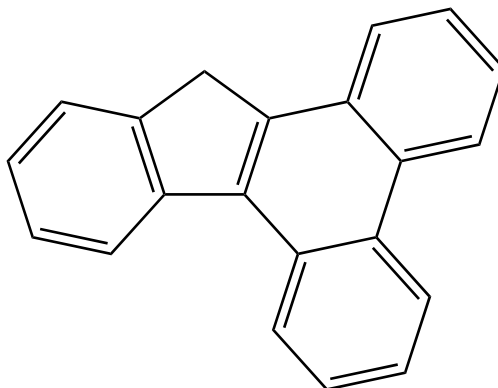
Cartesian coordinates:

C	-2.9047	1.6205	0.4637	C	1.2870	1.9893	-0.1348	H	-2.6794	-3.4874	-1.0540
C	-3.0061	0.1580	0.1550	C	2.6762	2.0821	-0.4987	H	-4.9031	-2.5717	-0.4625
C	-1.7201	-0.3805	-0.1006	C	3.4386	0.9725	-0.6216	H	-5.1326	-0.1908	0.2569
C	-1.6096	-1.6807	-0.5727	C	1.5618	-0.4310	0.1370	H	-1.3863	4.0377	0.4872
C	-2.7634	-2.4564	-0.6942	C	2.9106	-0.3115	-0.2507	H	1.0521	4.1415	-0.0563
C	-4.0131	-1.9406	-0.3726	C	3.7648	-1.4321	-0.1912	H	3.0914	3.0767	-0.6995
C	-4.1468	-0.6144	0.0416	C	3.3102	-2.6260	0.3222	H	4.4807	1.0318	-0.9553
C	-0.7256	0.6874	0.0854	C	2.0023	-2.7171	0.8205	H	4.7985	-1.3355	-0.5424
C	-1.4355	1.8822	0.3035	C	1.1483	-1.6390	0.7359	H	3.9700	-3.4984	0.3669
C	-0.8083	3.1261	0.3075	H	-3.5149	2.2289	-0.2291	H	1.6650	-3.6495	1.2850
C	0.5429	3.1747	0.0299	H	-3.2476	1.8565	1.4883	H	0.1412	-1.7039	1.1684
C	0.6840	0.7176	0.0195	H	-0.6379	-2.0941	-0.8681				

Table 3.87: Table of thermodynamic data as a function of temperature for 9*H*-Indeno[2,1-*c*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-40.912	356.707	356.707	∞
100	90.923	322.949	673.981	-35.103	380.691	420.904	-219.853
200	175.237	410.351	520.417	-22.013	368.077	466.128	-121.738
250	225.025	454.751	502.824	-12.018	362.084	491.335	-102.657
298.15	274.127	498.587	498.587	0.000	356.707	516.728	-90.527
300	275.999	500.289	498.592	0.509	356.509	517.720	-90.141
350	325.384	546.577	502.135	15.555	351.521	544.994	-81.334
400	371.378	593.073	510.597	32.990	347.166	572.931	-74.816
450	413.150	639.269	522.332	52.622	343.382	601.382	-69.805
500	450.557	684.773	536.308	74.232	340.101	630.245	-65.840
600	513.446	772.702	568.443	122.555	334.783	688.801	-59.964
700	563.389	855.744	603.615	176.490	330.919	748.133	-55.825
800	603.640	933.695	640.056	234.911	328.328	807.917	-52.751
900	636.603	1006.759	676.785	296.976	326.840	867.955	-50.374
1000	663.956	1075.291	713.245	362.045	326.298	928.116	-48.479
1100	686.885	1139.679	749.115	429.620	326.526	988.300	-46.929
1200	706.261	1200.300	784.213	499.304	327.393	1048.420	-45.636
1300	722.741	1257.499	818.441	570.776	328.739	1108.456	-44.537
1400	736.842	1311.589	851.751	643.773	330.448	1168.378	-43.592
1500	748.971	1362.850	884.131	718.079	332.443	1228.168	-42.768
1600	759.458	1411.530	915.585	793.513	334.615	1287.811	-42.042
1700	768.567	1457.852	946.132	869.925	336.897	1347.295	-41.396
1800	776.518	1502.012	975.797	947.188	339.225	1406.695	-40.820
1900	783.488	1544.187	1004.611	1025.196	341.570	1465.923	-40.300
2000	789.625	1584.534	1032.605	1103.858	343.883	1525.049	-39.829
2100	795.050	1623.194	1059.815	1183.097	346.101	1584.049	-39.400
2200	799.864	1660.293	1086.272	1262.847	348.222	1642.950	-39.008
2300	804.154	1695.945	1112.009	1343.052	350.237	1701.754	-38.647
2400	807.989	1730.252	1137.059	1423.663	352.090	1760.437	-38.314
2500	811.429	1763.307	1161.452	1504.637	353.789	1819.135	-38.008
2600	814.526	1795.193	1185.217	1585.937	355.304	1877.677	-37.722
2700	817.322	1825.987	1208.382	1667.532	356.636	1936.218	-37.458
2800	819.854	1855.757	1230.974	1749.393	357.766	1994.735	-37.211
2900	822.154	1884.568	1253.018	1831.495	358.669	2053.171	-36.981
3000	824.247	1912.476	1274.537	1913.817	359.377	2111.600	-36.765
3100	826.158	1939.534	1295.554	1996.338	359.831	2169.951	-36.563
3200	827.908	1965.792	1316.091	2079.043	360.061	2228.347	-36.373
3300	829.512	1991.293	1336.167	2161.915	360.054	2286.769	-36.196
3400	830.987	2016.078	1355.802	2244.941	359.787	2345.130	-36.028
3500	832.345	2040.187	1375.013	2328.109	359.262	2403.487	-35.869
3600	833.600	2063.652	1393.817	2411.407	358.497	2461.929	-35.721
3700	834.760	2086.508	1412.231	2494.825	357.468	2520.413	-35.581
3800	835.835	2108.784	1430.269	2578.356	356.151	2578.877	-35.448
3900	836.833	2130.508	1447.947	2661.990	354.581	2637.343	-35.323
4000	837.760	2151.707	1465.277	2745.720	352.743	2695.959	-35.205
4100	838.625	2172.404	1482.273	2829.540	350.610	2754.566	-35.093
4200	839.431	2192.623	1498.946	2913.443	348.203	2813.222	-34.987
4300	840.184	2212.384	1515.309	2997.424	345.511	2871.868	-34.886
4400	840.888	2231.708	1531.372	3081.478	342.541	2930.653	-34.791
4500	841.548	2250.612	1547.145	3165.600	339.303	2989.554	-34.701
4600	842.167	2269.115	1562.640	3249.786	335.758	3048.532	-34.616
4700	842.749	2287.234	1577.865	3334.033	331.916	3107.503	-34.535
4800	843.296	2304.982	1592.829	3418.335	327.815	3166.641	-34.459
4900	843.811	2322.376	1607.541	3502.691	323.397	3225.762	-34.386
5000	844.296	2339.428	1622.008	3587.096	318.735	3285.126	-34.319

3.88. 1*H*-Indeno[1,2-*l*]phenanthrene



Other names: 1*H*-Dibenzo[*a,c*]fluorene
1,2,3,4-Dibenzofluorene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 201-65-0

Point Group: C_s

Length: 13.36 Å

Width: 10.45 Å

Breadth: 4.178 Å

L/B Ratio: 1.279

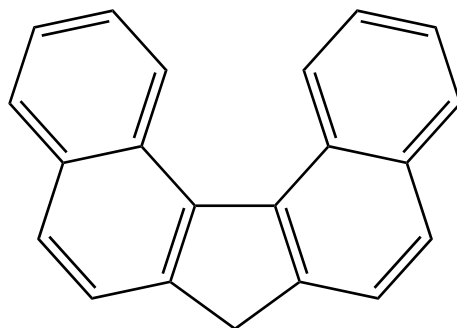
Cartesian coordinates:

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C	-2.0317	-0.5620	0.0000	C	2.4271	3.5172	0.0000	H	-4.7819	-2.5394	-0.0000
C	-2.6839	0.6961	0.0000	C	1.1501	3.0069	0.0000	H	-2.3079	-2.7125	-0.0000
C	-4.0631	0.7922	0.0000	C	1.8311	-0.6980	0.0000	H	4.2056	0.6026	0.0000
C	-4.8102	-0.3865	0.0000	C	0.5242	-1.2334	0.0000	H	4.5445	3.0660	-0.0000
C	-4.1788	-1.6254	-0.0000	C	0.3601	-2.6354	0.0000	H	2.5911	4.5996	0.0000
C	-2.7875	-1.7253	-0.0000	C	1.4494	-3.4755	0.0000	H	0.2814	3.6754	0.0000
C	-0.3698	1.0439	0.0000	C	2.7486	-2.9449	0.0000	H	-0.6529	-3.0596	0.0000
C	-0.5826	-0.3208	0.0000	C	2.9328	-1.5822	0.0000	H	1.3095	-4.5614	0.0000
C	0.9398	1.6105	0.0000	H	-1.7668	2.4497	0.8893	H	3.6101	-3.6204	0.0000
C	2.0429	0.7349	0.0000	H	-1.7668	2.4497	-0.8893	H	3.9482	-1.1570	0.0000
C	3.3434	1.2868	0.0000	H	-4.5561	1.7690	0.0000				

Table 3.88: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[1,2-*l*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.567	334.212	334.212	∞
100	93.794	335.449	689.371	-35.392	357.906	396.870	-207.299
200	176.632	424.434	534.846	-22.082	345.512	440.747	-115.109
250	225.687	469.063	517.210	-12.037	339.570	465.243	-97.205
298.15	274.265	512.969	512.969	0.000	334.212	489.945	-85.835
300	276.121	514.671	512.974	0.509	334.014	490.910	-85.473
350	325.139	560.949	516.517	15.551	329.022	517.465	-77.226
400	370.900	607.395	524.974	32.968	324.648	544.684	-71.127
450	412.530	653.526	536.700	52.572	320.837	572.421	-66.444
500	449.855	698.960	550.661	74.149	317.522	600.572	-62.740
600	512.679	786.754	582.757	122.398	312.130	657.717	-57.258
700	562.619	869.677	617.883	176.256	308.189	715.650	-53.401
800	602.889	947.526	654.275	234.601	305.521	774.046	-50.539
900	635.882	1020.503	690.957	296.592	303.960	832.705	-48.328
1000	663.270	1088.961	727.370	361.591	303.347	891.496	-46.566
1100	686.237	1153.286	763.196	429.099	303.509	950.316	-45.126
1200	705.651	1213.852	798.252	498.720	304.313	1009.078	-43.923
1300	722.171	1271.004	832.440	570.133	305.599	1067.761	-42.902
1400	736.309	1325.053	865.714	643.075	307.253	1126.335	-42.023
1500	748.475	1376.278	898.059	717.329	309.198	1184.780	-41.257
1600	758.995	1424.928	929.481	792.715	311.322	1243.082	-40.582
1700	768.137	1471.222	959.997	869.082	313.559	1301.228	-39.981
1800	776.118	1515.359	989.634	946.304	315.845	1359.292	-39.445
1900	783.115	1557.513	1018.422	1024.273	318.152	1417.186	-38.960
2000	789.277	1597.841	1046.392	1102.899	320.429	1474.980	-38.522
2100	794.725	1636.485	1073.578	1182.105	322.613	1532.651	-38.122
2200	799.561	1673.569	1100.013	1261.824	324.702	1590.224	-37.756
2300	803.870	1709.208	1125.730	1341.999	326.688	1647.700	-37.420
2400	807.723	1743.503	1150.760	1422.582	328.514	1705.058	-37.109
2500	811.180	1776.547	1175.135	1503.531	330.187	1762.432	-36.823
2600	814.292	1808.424	1198.883	1584.807	331.678	1819.650	-36.556
2700	817.102	1839.209	1222.032	1666.379	332.988	1876.869	-36.309
2800	819.647	1868.972	1244.608	1748.219	334.096	1934.063	-36.080
2900	821.958	1897.776	1266.637	1830.301	334.978	1991.178	-35.864
3000	824.063	1925.677	1288.143	1912.603	335.668	2048.286	-35.663
3100	825.984	1952.730	1309.147	1995.107	336.104	2105.317	-35.474
3200	827.743	1978.982	1329.671	2077.795	336.318	2162.394	-35.297
3300	829.355	2004.478	1349.735	2160.651	336.294	2219.498	-35.131
3400	830.838	2029.259	1369.359	2243.662	336.011	2276.540	-34.974
3500	832.204	2053.363	1388.559	2326.815	335.472	2333.580	-34.826
3600	833.466	2076.825	1407.353	2410.099	334.694	2390.704	-34.688
3700	834.632	2099.677	1425.757	2493.505	333.651	2447.871	-34.557
3800	835.713	2121.950	1443.786	2577.023	332.322	2505.018	-34.433
3900	836.717	2143.671	1461.454	2660.645	330.740	2562.168	-34.316
4000	837.650	2164.867	1478.776	2744.364	328.891	2619.468	-34.206
4100	838.519	2185.561	1495.763	2828.172	326.747	2676.759	-34.102
4200	839.329	2205.777	1512.429	2912.065	324.330	2734.099	-34.003
4300	840.087	2225.536	1528.784	2996.037	321.627	2791.430	-33.908
4400	840.795	2244.858	1544.839	3080.081	318.648	2848.900	-33.820
4500	841.459	2263.760	1560.606	3164.194	315.401	2906.486	-33.737
4600	842.082	2282.261	1576.094	3248.371	311.847	2964.150	-33.658
4700	842.667	2300.378	1591.312	3332.609	307.997	3021.806	-33.583
4800	843.217	2318.125	1606.270	3416.904	303.888	3079.629	-33.513
4900	843.735	2335.517	1620.975	3501.252	299.462	3137.437	-33.445
5000	844.223	2352.567	1635.437	3585.650	294.792	3195.486	-33.382

3.89. 7H-Dibenzo[*c,g*]fluorene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 194-58-1
Point Group: C₂

Length: 12.67 Å
Width: 9.700 Å
Breadth: 5.021 Å
L/B Ratio: 1.306

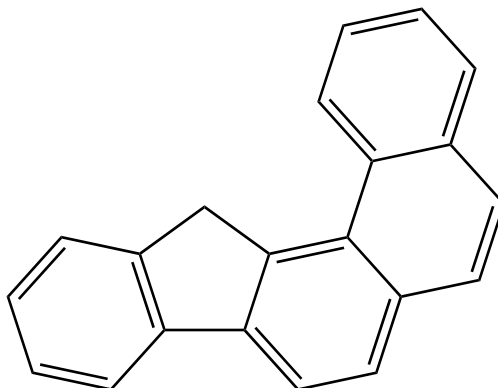
Cartesian coordinates:

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C	1.1543	-1.9964	0.1433	C	-2.4934	-2.3633	-0.3486	H	0.4520	1.9602	-0.7670
C	0.7380	-0.6658	0.0295	C	-3.4423	-1.3767	-0.3956	H	2.2663	3.6259	-0.9160
C	3.4423	-1.3767	0.3956	C	-1.7357	0.3447	0.0837	H	4.5970	3.0130	-0.3169
C	2.4934	-2.3633	0.3486	C	-3.0854	-0.0240	-0.1484	H	5.1385	0.6695	0.3131
C	3.0854	-0.0240	0.1484	C	-4.1074	0.9637	-0.0856	H	-2.7554	-3.4184	-0.4745
C	1.7357	0.3447	-0.0837	C	-3.8124	2.2514	0.2665	H	-4.4926	-1.6212	-0.5910
C	1.4791	1.6784	-0.4992	C	-2.4829	2.6037	0.5884	H	-5.1385	0.6695	-0.3131
C	2.4829	2.6037	-0.5884	C	-1.4791	1.6784	0.4992	H	-4.5970	3.0130	0.3169
C	3.8124	2.2514	-0.2665	H	0.1216	-3.5959	-0.8805	H	-2.2663	3.6259	0.9160
C	4.1074	0.9637	0.0856	H	-0.1216	-3.5959	0.8805	H	-0.4520	1.9602	0.7671
C	-0.7380	-0.6658	-0.0295	H	4.4926	-1.6212	0.5910				

Table 3.89: Table of thermodynamic data as a function of temperature for 7*H*-Dibenzo[*c,g*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-40.917	364.151	364.151	∞
100	90.726	316.959	668.268	-35.131	388.107	428.919	-224.040
200	175.441	404.366	514.555	-22.038	375.496	474.744	-123.988
250	225.286	448.819	496.942	-12.031	369.515	500.248	-104.519
298.15	274.379	492.701	492.701	0.000	364.151	525.926	-92.138
300	276.250	494.405	492.707	0.509	363.953	526.929	-91.745
350	325.598	540.729	496.253	15.567	358.976	554.496	-82.752
400	371.554	587.251	504.720	33.012	354.631	582.724	-76.094
450	413.293	633.466	516.463	52.652	350.855	611.467	-70.976
500	450.674	678.983	530.446	74.269	347.580	640.619	-66.924
600	513.528	766.931	562.595	122.602	342.272	699.753	-60.918
700	563.449	849.984	597.779	176.543	338.415	759.662	-56.685
800	603.685	927.941	634.229	234.970	335.829	820.022	-53.541
900	636.638	1001.010	670.967	297.039	334.345	880.634	-51.110
1000	663.983	1069.545	707.434	362.111	333.806	941.370	-49.171
1100	686.907	1133.936	743.310	429.688	334.037	1002.129	-47.586
1200	706.278	1194.558	778.413	499.374	334.906	1062.823	-46.263
1300	722.755	1251.759	812.645	570.847	336.253	1123.433	-45.139
1400	736.853	1305.850	845.960	643.846	337.963	1183.929	-44.172
1500	748.980	1357.111	878.343	718.153	339.960	1244.293	-43.329
1600	759.465	1405.792	909.800	793.587	342.133	1304.510	-42.587
1700	768.573	1452.114	940.350	870.000	344.415	1364.568	-41.927
1800	776.523	1496.275	970.017	947.263	346.744	1424.541	-41.338
1900	783.492	1538.450	998.833	1025.272	349.089	1484.343	-40.807
2000	789.628	1578.797	1026.830	1103.934	351.403	1544.043	-40.325
2100	795.052	1617.457	1054.041	1183.174	353.621	1603.617	-39.887
2200	799.867	1654.556	1080.500	1262.924	355.742	1663.091	-39.486
2300	804.156	1690.208	1106.239	1343.129	357.757	1722.469	-39.118
2400	807.991	1724.515	1131.290	1423.740	359.611	1781.726	-38.777
2500	811.431	1757.570	1155.684	1504.714	361.310	1840.998	-38.465
2600	814.528	1789.456	1179.450	1586.015	362.824	1900.113	-38.173
2700	817.323	1820.250	1202.617	1667.610	364.157	1959.228	-37.903
2800	819.855	1850.021	1225.210	1749.471	365.287	2018.319	-37.651
2900	822.154	1878.831	1247.254	1831.573	366.190	2077.328	-37.416
3000	824.248	1906.739	1268.774	1913.895	366.898	2136.330	-37.196
3100	826.159	1933.798	1289.793	1996.417	367.352	2195.255	-36.989
3200	827.908	1960.055	1310.330	2079.121	367.583	2254.225	-36.796
3300	829.512	1985.556	1330.407	2161.993	367.575	2313.220	-36.614
3400	830.987	2010.342	1350.042	2245.019	367.308	2372.155	-36.443
3500	832.346	2034.450	1369.254	2328.187	366.784	2431.086	-36.281
3600	833.600	2057.916	1388.059	2411.485	366.019	2490.102	-36.130
3700	834.760	2080.772	1406.473	2494.904	364.989	2549.160	-35.987
3800	835.835	2103.048	1424.512	2578.434	363.673	2608.197	-35.851
3900	836.833	2124.772	1442.190	2662.068	362.103	2667.237	-35.723
4000	837.761	2145.971	1459.521	2745.799	360.265	2726.426	-35.603
4100	838.625	2166.668	1476.517	2829.618	358.132	2785.607	-35.488
4200	839.431	2186.886	1493.191	2913.522	355.725	2844.836	-35.380
4300	840.184	2206.648	1509.554	2997.503	353.032	2904.056	-35.277
4400	840.888	2225.971	1525.617	3081.557	350.062	2963.415	-35.179
4500	841.548	2244.876	1541.392	3165.679	346.824	3022.890	-35.088
4600	842.168	2263.379	1556.887	3249.865	343.280	3082.441	-35.002
4700	842.749	2281.497	1572.112	3334.111	339.438	3141.986	-34.919
4800	843.296	2299.246	1587.076	3418.414	335.337	3201.697	-34.841
4900	843.811	2316.639	1601.788	3502.769	330.919	3261.392	-34.766
5000	844.296	2333.691	1616.256	3587.175	326.256	3321.329	-34.697

3.90. 1*H*-Indeno[1,2-*c*]phenanthrene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 212-54-4
Point Group: C_s

Length: 14.01 Å
Width: 9.692 Å
Breadth: 4.167 Å
L/B Ratio: 1.445

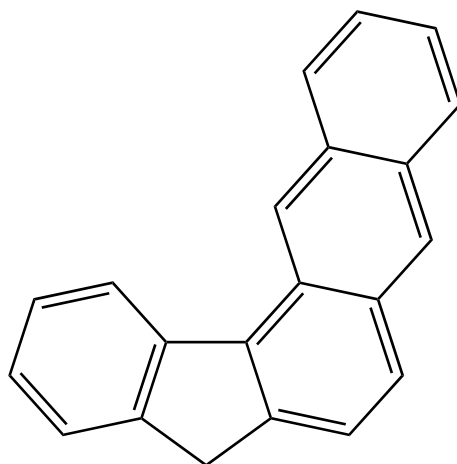
Cartesian coordinates:

C	1.2174	-1.1417	0.0000	C	-1.3978	1.7017	0.0000	H	5.9614	-1.3341	-0.0000
C	2.6963	0.7259	0.0000	C	-2.8027	2.0059	0.0000	H	6.0512	1.1370	-0.0000
C	2.6450	-0.6864	0.0000	C	-3.7276	1.0210	0.0000	H	3.9483	2.4868	-0.0000
C	3.8071	-1.4352	0.0000	C	-1.9583	-0.7006	0.0000	H	1.5965	3.3786	-0.0000
C	5.0295	-0.7590	-0.0000	C	-3.3253	-0.3575	0.0000	H	-0.8666	3.8016	-0.0000
C	5.0800	0.6311	-0.0000	C	-4.3136	-1.3645	-0.0000	H	-3.1046	3.0600	0.0000
C	3.9103	1.3928	-0.0000	C	-3.9567	-2.6934	-0.0000	H	-4.7994	1.2507	-0.0000
C	0.4324	0.1455	0.0000	C	-2.5999	-3.0465	-0.0000	H	-5.3708	-1.0749	-0.0000
C	1.3252	1.2302	0.0000	C	-1.6261	-2.0727	0.0000	H	-4.7224	-3.4757	-0.0000
C	0.8787	2.5519	-0.0000	H	0.9699	-1.7646	0.8841	H	-2.3179	-4.1046	-0.0000
C	-0.4818	2.7749	0.0000	H	0.9699	-1.7646	-0.8841	H	-0.5667	-2.3751	0.0000
C	-0.9599	0.3546	0.0000	H	3.7715	-2.5287	0.0000				

Table 3.90: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[1,2-*c*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-40.897	329.875	329.875	∞
100	90.989	324.988	675.544	-35.056	353.907	393.916	-205.756
200	174.950	412.328	522.211	-21.977	341.282	438.937	-114.636
250	224.645	456.653	504.647	-11.999	335.272	464.047	-96.955
298.15	273.696	500.417	500.417	0.000	329.875	489.350	-85.730
300	275.566	502.116	500.423	0.508	329.676	490.339	-85.374
350	324.917	548.335	503.960	15.531	324.665	517.523	-77.234
400	370.891	594.767	512.410	32.943	320.286	545.373	-71.217
450	412.655	640.906	524.128	52.550	316.478	573.742	-66.597
500	450.063	686.357	538.086	74.136	313.172	602.524	-62.944
600	512.972	774.198	570.181	122.410	307.805	660.926	-57.538
700	562.946	857.169	605.313	176.299	303.895	720.112	-53.734
800	603.231	935.063	641.716	234.678	301.262	779.757	-50.912
900	636.228	1008.080	678.410	296.703	299.734	839.660	-48.732
1000	663.613	1076.575	714.838	361.737	299.157	899.691	-46.994
1100	686.571	1140.932	750.678	429.279	299.352	959.748	-45.574
1200	705.973	1201.526	785.749	498.933	300.189	1019.744	-44.387
1300	722.478	1258.703	819.952	570.377	301.507	1079.659	-43.380
1400	736.601	1312.775	853.240	643.349	303.191	1139.462	-42.513
1500	748.750	1364.020	885.599	717.631	305.163	1199.134	-41.757
1600	759.254	1412.686	917.034	793.044	307.314	1258.661	-41.090
1700	768.380	1458.996	947.563	869.436	309.576	1318.030	-40.497
1800	776.345	1503.146	977.212	946.681	311.887	1377.316	-39.968
1900	783.328	1545.312	1006.011	1024.673	314.215	1436.431	-39.489
2000	789.477	1585.651	1033.991	1103.319	316.512	1495.444	-39.056
2100	794.912	1624.304	1061.188	1182.544	318.716	1554.333	-38.661
2200	799.737	1661.397	1087.633	1262.281	320.823	1613.124	-38.300
2300	804.035	1697.043	1113.359	1342.474	322.826	1671.817	-37.967
2400	807.878	1731.345	1138.398	1423.073	324.668	1730.391	-37.660
2500	811.326	1764.396	1162.781	1504.036	326.357	1788.980	-37.378
2600	814.429	1796.278	1186.537	1585.327	327.861	1847.413	-37.114
2700	817.231	1827.068	1209.693	1666.912	329.184	1905.846	-36.870
2800	819.769	1856.836	1232.277	1748.764	330.305	1964.255	-36.643
2900	822.073	1885.643	1254.313	1830.858	331.199	2022.583	-36.430
3000	824.172	1913.549	1275.825	1913.172	331.900	2080.904	-36.231
3100	826.087	1940.605	1296.835	1995.687	332.347	2139.148	-36.044
3200	827.840	1966.860	1317.365	2078.384	332.570	2197.437	-35.869
3300	829.448	1992.359	1337.435	2161.250	332.556	2255.753	-35.705
3400	830.926	2017.143	1357.064	2244.269	332.283	2314.007	-35.550
3500	832.288	2041.249	1376.269	2327.431	331.752	2372.259	-35.403
3600	833.545	2064.713	1395.068	2410.724	330.982	2430.594	-35.266
3700	834.708	2087.568	1413.477	2494.137	329.947	2488.972	-35.137
3800	835.785	2109.842	1431.510	2577.662	328.625	2547.330	-35.015
3900	836.785	2131.565	1449.183	2661.291	327.051	2605.690	-34.899
4000	837.715	2152.763	1466.509	2745.017	325.208	2664.201	-34.790
4100	838.582	2173.459	1483.500	2828.832	323.071	2722.702	-34.687
4200	839.390	2193.677	1500.169	2912.731	320.660	2781.253	-34.589
4300	840.144	2213.437	1516.528	2996.709	317.963	2839.793	-34.496
4400	840.851	2232.759	1532.587	3080.759	314.989	2898.473	-34.409
4500	841.512	2251.663	1548.357	3164.877	311.747	2957.269	-34.326
4600	842.133	2270.166	1563.848	3249.060	308.199	3016.143	-34.249
4700	842.716	2288.283	1579.070	3333.303	304.354	3075.008	-34.174
4800	843.264	2306.031	1594.030	3417.602	300.250	3134.041	-34.105
4900	843.780	2323.424	1608.739	3501.954	295.828	3193.058	-34.038
5000	844.267	2340.475	1623.204	3586.357	291.163	3252.316	-33.976

3.91. 8*H*-Indeno[1,2-*a*]anthracene



Other names: 8*H*-Naphtho[2,3-*c*]fluorene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 198-95-8

Point Group: C_s

Length: 14.24 Å

Width: 9.874 Å

Breadth: 4.177 Å

L/B Ratio: 1.442

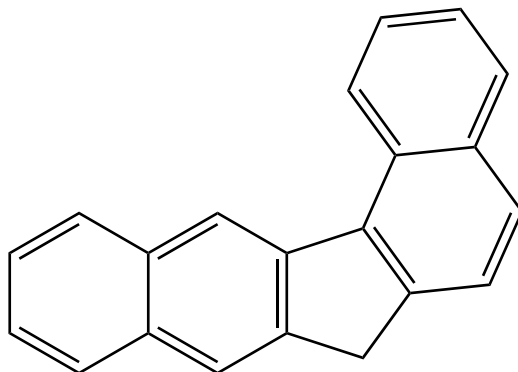
Cartesian coordinates:

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C	3.4333	0.4194	-0.0000	C	-2.5325	1.4090	0.0000	H	5.6675	-2.1173	-0.0000
C	2.2298	-0.3296	0.0000	C	-0.8957	-0.8657	0.0000	H	5.5908	0.3772	-0.0000
C	2.2788	-1.7156	0.0000	C	-2.2839	-1.0118	0.0000	H	1.2421	4.0407	-0.0000
C	3.5246	-2.3434	0.0000	C	-3.1148	0.1409	0.0000	H	-1.2357	3.7340	0.0000
C	4.7012	-1.6025	0.0000	C	-4.5382	-0.0288	0.0000	H	-3.1741	2.2992	0.0000
C	4.6655	-0.2069	-0.0000	C	-5.0843	-1.2739	-0.0000	H	-0.2602	-1.7638	0.0000
C	1.1076	0.6146	0.0000	C	-4.2511	-2.4308	-0.0000	H	-5.1698	0.8667	0.0000
C	1.6235	1.9018	0.0000	C	-2.8969	-2.3078	0.0000	H	-6.1706	-1.4102	-0.0000
C	0.7900	3.0440	0.0000	H	3.5401	2.3972	0.8891	H	-4.7246	-3.4179	-0.0000
C	-0.5618	2.8693	0.0000	H	3.5401	2.3972	-0.8891	H	-2.2485	-3.1912	-0.0000
C	-0.3062	0.4010	0.0000	H	1.3563	-2.3111	0.0000				

Table 3.91: Table of thermodynamic data as a function of temperature for 8*H*-Indeno[1,2-*a*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.391	346.571	346.571	∞
100	92.296	330.833	684.484	-35.365	370.293	409.718	-214.010
200	176.589	419.168	529.870	-22.141	357.813	454.101	-118.597
250	226.336	463.866	512.181	-12.079	351.887	478.859	-100.050
298.15	275.314	507.924	507.924	0.000	346.571	503.808	-88.263
300	277.180	509.633	507.929	0.511	346.375	504.783	-87.889
350	326.378	556.090	511.486	15.611	341.441	531.585	-79.333
400	372.178	602.705	519.976	33.092	337.131	559.043	-73.002
450	413.773	648.986	531.744	52.759	333.383	587.010	-68.137
500	451.033	694.547	545.754	74.397	330.129	615.386	-64.288
600	513.715	782.543	577.950	122.756	324.847	672.960	-58.585
700	563.536	865.617	613.172	176.711	321.003	731.307	-54.570
800	603.718	943.582	649.653	235.143	318.423	790.103	-51.587
900	636.642	1016.653	686.415	297.214	316.941	849.152	-49.282
1000	663.973	1085.187	722.902	362.286	316.402	908.323	-47.445
1100	686.890	1149.577	758.794	429.861	316.630	967.517	-45.943
1200	706.258	1210.197	793.910	499.545	317.497	1026.648	-44.688
1300	722.735	1267.396	828.153	571.017	318.843	1085.694	-43.623
1400	736.834	1321.486	861.477	644.013	320.551	1144.626	-42.706
1500	748.962	1372.746	893.867	718.318	322.546	1203.427	-41.906
1600	759.448	1421.426	925.331	793.751	324.717	1262.080	-41.202
1700	768.558	1467.747	955.887	870.162	326.998	1320.575	-40.575
1800	776.508	1511.906	985.560	947.424	329.325	1378.985	-40.016
1900	783.479	1554.081	1014.380	1025.431	331.669	1437.224	-39.511
2000	789.616	1594.427	1042.381	1104.092	333.981	1495.360	-39.054
2100	795.041	1633.087	1069.596	1183.330	336.198	1553.371	-38.637
2200	799.857	1670.186	1096.058	1263.080	338.318	1611.283	-38.256
2300	804.147	1705.837	1121.800	1343.284	340.332	1669.097	-37.906
2400	807.982	1740.144	1146.855	1423.894	342.185	1726.791	-37.582
2500	811.423	1773.198	1171.251	1504.867	343.883	1784.500	-37.284
2600	814.520	1805.084	1195.020	1586.167	345.397	1842.053	-37.007
2700	817.317	1835.878	1218.188	1667.761	346.729	1899.605	-36.749
2800	819.849	1865.648	1240.783	1749.622	347.859	1957.133	-36.510
2900	822.149	1894.458	1262.830	1831.723	348.760	2014.580	-36.286
3000	824.242	1922.366	1284.352	1914.044	349.468	2072.019	-36.076
3100	826.154	1949.425	1305.371	1996.566	349.922	2129.381	-35.879
3200	827.903	1975.682	1325.910	2079.270	350.152	2186.788	-35.695
3300	829.508	2001.183	1345.989	2162.142	350.144	2244.221	-35.522
3400	830.983	2025.968	1365.625	2245.167	349.876	2301.593	-35.359
3500	832.342	2050.076	1384.838	2328.334	349.351	2358.962	-35.205
3600	833.596	2073.542	1403.644	2411.632	348.586	2416.415	-35.061
3700	834.757	2096.398	1422.060	2495.050	347.556	2473.910	-34.925
3800	835.832	2118.674	1440.100	2578.580	346.239	2531.385	-34.796
3900	836.830	2140.398	1457.779	2662.214	344.669	2588.862	-34.673
4000	837.758	2161.596	1475.110	2745.944	342.831	2646.489	-34.559
4100	838.622	2182.294	1492.107	2829.764	340.698	2704.107	-34.450
4200	839.428	2202.512	1508.782	2913.667	338.290	2761.774	-34.347
4300	840.181	2222.273	1525.146	2997.647	335.597	2819.431	-34.249
4400	840.886	2241.597	1541.210	3081.701	332.627	2877.227	-34.156
4500	841.546	2260.501	1556.985	3165.823	329.389	2935.139	-34.070
4600	842.165	2279.004	1572.481	3250.009	325.844	2993.129	-33.987
4700	842.747	2297.123	1587.707	3334.255	322.002	3051.111	-33.909
4800	843.294	2314.871	1602.672	3418.557	317.901	3109.259	-33.835
4900	843.809	2332.265	1617.384	3502.913	313.483	3167.392	-33.764
5000	844.295	2349.317	1631.853	3587.318	308.820	3225.767	-33.699

3.92. 7H-Dibenzo[b,g]fluorene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 204-89-7
Point Group: C_s

Length: 14.33 Å
Width: 9.541 Å
Breadth: 4.177 Å
L/B Ratio: 1.502

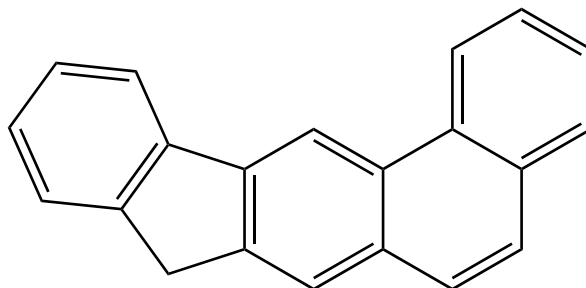
Cartesian coordinates:

C	0.0338	2.6491	-0.0000	C	-1.2713	1.9071	0.0000	H	2.9151	2.5957	0.0000
C	1.0442	1.5402	0.0000	C	-2.5562	2.4715	0.0000	H	2.7822	-2.9832	0.0000
C	0.3710	0.2676	0.0000	C	-3.6437	1.6345	0.0000	H	5.2640	-2.8607	0.0000
C	1.0918	-0.8929	0.0000	C	-2.1855	-0.3527	0.0000	H	6.4098	-0.6634	0.0000
C	2.4030	1.6275	0.0000	C	-3.4795	0.2239	0.0000	H	5.0881	1.4420	0.0000
C	3.1689	0.4246	0.0000	C	-4.6210	-0.6262	0.0000	H	-2.6734	3.5597	0.0000
C	2.5153	-0.8266	0.0000	C	-4.4757	-1.9854	0.0000	H	-4.6594	2.0467	0.0000
C	3.2943	-2.0143	0.0000	C	-3.1842	-2.5625	0.0000	H	-5.6176	-0.1701	0.0000
C	4.6621	-1.9462	0.0000	C	-2.0701	-1.7698	0.0000	H	-5.3525	-2.6411	0.0000
C	5.3154	-0.6934	0.0000	H	0.1348	3.2994	0.8887	H	-3.0899	-3.6534	-0.0000
C	4.5878	0.4670	0.0000	H	0.1348	3.2994	-0.8887	H	-1.0687	-2.2218	0.0000
C	-1.0730	0.5265	0.0000	H	0.6002	-1.8759	0.0000				

Table 3.92: Table of thermodynamic data as a function of temperature for 7*H*-Dibenzo[*b,g*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.132	331.084	331.084	∞
100	91.540	329.211	680.955	-35.174	354.996	394.583	-206.105
200	175.612	416.964	527.139	-22.035	342.432	439.160	-114.694
250	225.250	461.432	509.532	-12.025	336.454	464.034	-96.953
298.15	274.175	505.293	505.293	0.000	331.084	489.105	-85.687
300	276.040	506.995	505.299	0.509	330.885	490.085	-85.330
350	325.237	553.276	508.841	15.552	325.895	517.023	-77.160
400	371.070	599.741	517.300	32.976	321.528	544.625	-71.119
450	412.721	645.894	529.029	52.589	317.725	572.745	-66.481
500	450.047	691.347	542.996	74.176	314.420	601.277	-62.814
600	512.866	779.176	575.103	122.444	309.047	659.181	-57.386
700	562.814	862.128	610.242	176.320	305.125	717.871	-53.567
800	603.103	940.004	646.647	234.685	302.478	777.020	-50.733
900	636.116	1013.008	683.342	296.699	300.939	836.430	-48.544
1000	663.520	1081.491	719.769	361.722	300.351	895.969	-46.800
1100	686.497	1145.840	755.607	429.256	300.537	955.535	-45.374
1200	705.915	1206.429	790.676	498.903	301.368	1015.040	-44.183
1300	722.434	1263.602	824.877	570.342	302.681	1074.465	-43.172
1400	736.567	1317.671	858.163	643.311	304.361	1133.777	-42.301
1500	748.725	1368.914	890.520	717.590	306.331	1192.960	-41.542
1600	759.235	1417.579	921.953	793.001	308.479	1251.998	-40.873
1700	768.367	1463.887	952.481	869.391	310.740	1310.878	-40.278
1800	776.336	1508.037	982.128	946.635	313.049	1369.674	-39.746
1900	783.322	1550.202	1010.926	1024.626	315.376	1428.301	-39.266
2000	789.473	1590.541	1038.905	1103.272	317.673	1486.825	-38.831
2100	794.911	1629.194	1066.100	1182.497	319.877	1545.225	-38.435
2200	799.737	1666.287	1092.544	1262.234	321.984	1603.526	-38.072
2300	804.036	1701.933	1118.270	1342.426	323.987	1661.731	-37.738
2400	807.880	1736.235	1143.308	1423.026	325.829	1719.816	-37.430
2500	811.328	1769.286	1167.690	1503.989	327.518	1777.916	-37.147
2600	814.432	1801.168	1191.445	1585.280	329.022	1835.860	-36.882
2700	817.235	1831.958	1214.601	1666.865	330.346	1893.804	-36.637
2800	819.772	1861.726	1237.184	1748.718	331.467	1951.724	-36.409
2900	822.077	1890.534	1259.219	1830.812	332.362	2009.563	-36.195
3000	824.175	1918.439	1280.731	1913.126	333.063	2067.395	-35.996
3100	826.091	1945.496	1301.740	1995.641	333.510	2125.150	-35.808
3200	827.844	1971.751	1322.270	2078.339	333.734	2182.950	-35.632
3300	829.452	1997.250	1342.339	2161.205	333.720	2240.776	-35.468
3400	830.930	2022.034	1361.968	2244.225	333.447	2298.542	-35.312
3500	832.292	2046.140	1381.173	2327.387	332.917	2356.304	-35.165
3600	833.549	2069.605	1399.971	2410.680	332.147	2414.150	-35.028
3700	834.712	2092.459	1418.380	2494.094	331.112	2472.039	-34.898
3800	835.789	2114.734	1436.413	2577.620	329.791	2529.908	-34.775
3900	836.789	2136.457	1454.085	2661.249	328.217	2587.779	-34.659
4000	837.719	2157.655	1471.411	2744.975	326.375	2645.800	-34.550
4100	838.585	2178.351	1488.402	2828.791	324.237	2703.812	-34.446
4200	839.393	2198.569	1505.071	2912.690	321.827	2761.873	-34.348
4300	840.148	2218.329	1521.429	2996.668	319.130	2819.925	-34.255
4400	840.854	2237.652	1537.488	3080.718	316.157	2878.116	-34.167
4500	841.515	2256.555	1553.258	3164.837	312.916	2936.423	-34.084
4600	842.136	2275.058	1568.749	3249.020	309.367	2994.807	-34.006
4700	842.719	2293.175	1583.970	3333.263	305.522	3053.183	-33.932
4800	843.267	2310.923	1598.931	3417.562	301.419	3111.727	-33.862
4900	843.783	2328.316	1613.640	3501.915	296.998	3170.254	-33.795
5000	844.270	2345.368	1628.104	3586.318	292.333	3229.024	-33.733

3.93. 8*H*-Indeno[2,1-*b*]phenanthrene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 241-28-1
Point Group: C_s

Length: 14.82 Å
Width: 9.283 Å
Breadth: 4.176 Å
L/B Ratio: 1.596

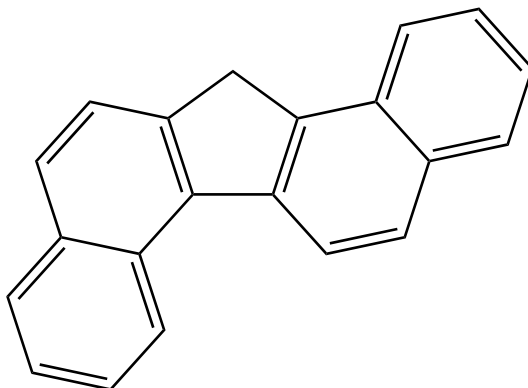
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C	3.1327	-1.7537	-0.0000	C	-2.4061	-0.5087	-0.0000	H	0.2217	3.3187	0.0000
C	4.5162	-1.9451	-0.0000	C	-3.5784	0.2676	0.0000	H	0.0246	-1.7085	-0.0000
C	5.3873	-0.8620	0.0000	C	-4.8385	-0.3704	0.0000	H	-2.2039	3.4083	-0.0000
C	4.9051	0.4500	0.0000	C	-4.9219	-1.7435	0.0000	H	-4.4139	2.2808	0.0000
C	1.2811	0.0517	-0.0000	C	-3.7519	-2.5224	0.0000	H	-5.7470	0.2424	0.0000
C	1.3374	1.4791	0.0000	C	-2.5172	-1.9168	0.0000	H	-5.8983	-2.2388	0.0000
C	0.1894	2.2238	0.0000	H	3.0015	2.5543	0.8886	H	-3.8316	-3.6143	0.0000
C	0.0805	-0.6092	-0.0000	H	3.0015	2.5543	-0.8886	H	-1.5924	-2.5139	0.0000
C	-1.1175	0.1471	-0.0000	H	2.4450	-2.6053	-0.0000				

Table 3.93: Table of thermodynamic data as a function of temperature for 8*H*-Indeno[2,1-*b*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.219	316.911	316.911	∞
100	92.400	328.384	680.857	-35.247	340.751	380.420	-198.707
200	175.888	416.536	526.805	-22.054	328.240	425.054	-111.010
250	225.429	461.053	509.185	-12.033	322.273	449.948	-94.010
298.15	274.335	504.944	504.944	0.000	316.911	475.037	-83.223
300	276.200	506.646	504.949	0.509	316.713	476.017	-82.880
350	325.405	552.952	508.493	15.560	311.730	502.972	-75.063
400	371.251	599.440	516.957	32.993	307.372	530.590	-69.287
450	412.909	645.615	528.692	52.615	303.579	558.724	-64.854
500	450.238	691.089	542.665	74.212	300.284	587.270	-61.350
600	513.055	778.952	574.788	122.499	294.930	645.197	-56.168
700	562.999	861.933	609.942	176.394	291.026	703.908	-52.525
800	603.284	939.834	646.362	234.777	288.397	763.076	-49.823
900	636.293	1012.858	683.070	296.809	286.876	822.502	-47.736
1000	663.692	1081.360	719.510	361.850	286.305	882.054	-46.073
1100	686.663	1145.725	755.361	429.400	286.509	941.632	-44.713
1200	706.074	1206.328	790.442	499.064	287.356	1001.149	-43.578
1300	722.584	1263.514	824.653	570.518	288.684	1060.583	-42.614
1400	736.710	1317.593	857.950	643.501	290.379	1119.904	-41.783
1500	748.859	1368.846	890.316	717.795	292.362	1179.094	-41.059
1600	759.362	1417.519	921.758	793.218	294.524	1238.138	-40.420
1700	768.485	1463.835	952.294	869.621	296.797	1297.024	-39.852
1800	776.447	1507.991	981.949	946.877	299.117	1355.825	-39.344
1900	783.426	1550.163	1010.753	1024.878	301.456	1414.456	-38.885
2000	789.571	1590.507	1038.740	1103.534	303.763	1472.984	-38.470
2100	795.002	1629.164	1065.941	1182.768	305.976	1531.387	-38.090
2200	799.823	1666.261	1092.391	1262.514	308.092	1589.691	-37.743
2300	804.117	1701.911	1118.122	1342.715	310.103	1647.898	-37.424
2400	807.956	1736.217	1143.166	1423.322	311.953	1705.985	-37.129
2500	811.400	1769.270	1167.553	1504.293	313.649	1764.087	-36.858
2600	814.500	1801.155	1191.313	1585.591	315.161	1822.032	-36.604
2700	817.298	1831.948	1214.473	1667.183	316.491	1879.977	-36.370
2800	819.832	1861.718	1237.060	1749.042	317.619	1937.898	-36.151
2900	822.133	1890.528	1259.099	1831.142	318.519	1995.738	-35.946
3000	824.229	1918.435	1280.614	1913.462	319.225	2053.570	-35.755
3100	826.142	1945.493	1301.628	1995.981	319.677	2111.326	-35.575
3200	827.892	1971.750	1322.161	2078.684	319.906	2169.126	-35.407
3300	829.498	1997.250	1342.234	2161.555	319.897	2226.952	-35.249
3400	830.973	2022.036	1361.865	2244.580	319.628	2284.717	-35.100
3500	832.333	2046.143	1381.073	2327.746	319.103	2342.479	-34.959
3600	833.588	2069.609	1399.875	2411.043	318.337	2400.325	-34.827
3700	834.749	2092.464	1418.286	2494.460	317.306	2458.214	-34.703
3800	835.825	2114.740	1436.322	2577.990	315.989	2516.082	-34.585
3900	836.823	2136.464	1453.997	2661.623	314.418	2573.953	-34.474
4000	837.752	2157.662	1471.324	2745.352	312.579	2631.973	-34.369
4100	838.616	2178.359	1488.318	2829.171	310.445	2689.985	-34.270
4200	839.423	2198.578	1504.989	2913.073	308.037	2748.045	-34.176
4300	840.176	2218.339	1521.350	2997.054	305.344	2806.095	-34.087
4400	840.881	2237.662	1537.411	3081.107	302.373	2864.285	-34.003
4500	841.542	2256.567	1553.183	3165.228	299.134	2922.591	-33.924
4600	842.161	2275.070	1568.675	3249.414	295.589	2980.974	-33.849
4700	842.743	2293.188	1583.898	3333.659	291.746	3039.349	-33.778
4800	843.290	2310.936	1598.861	3417.961	287.645	3097.891	-33.711
4900	843.805	2328.329	1613.571	3502.316	283.226	3156.417	-33.647
5000	844.291	2345.382	1628.037	3586.721	278.563	3215.185	-33.588

3.94. 1*H*-Dibenzo[*a,g*]fluorene



Other names: 1,2,5,6-Dibenzofluorene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 207-83-0

Point Group: C_s

Length: 14.84 Å

Width: 9.183 Å

Breadth: 4.177 Å

L/B Ratio: 1.616

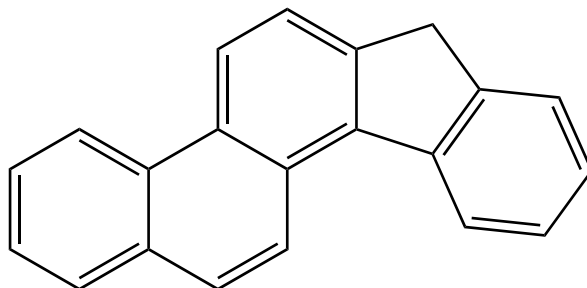
Cartesian coordinates:

C	-0.5867	-1.9873	-0.0000	C	-0.3050	0.3755	0.0000	H	4.1054	-2.6251	0.0000
C	1.0300	-0.2323	0.0000	C	-0.7095	1.7253	0.0000	H	5.6003	-0.7319	0.0000
C	0.8683	-1.6192	0.0000	C	-2.0480	2.0239	0.0000	H	5.9831	1.7230	0.0000
C	1.9641	-2.4963	0.0000	C	-2.6404	-0.3594	0.0000	H	4.0585	3.2860	-0.0000
C	3.2293	-1.9664	0.0000	C	-3.0325	0.9991	0.0000	H	1.7376	2.4258	-0.0000
C	2.3320	0.3313	0.0000	C	-4.4189	1.3159	0.0000	H	0.0442	2.5238	0.0000
C	3.4332	-0.5599	0.0000	C	-5.3569	0.3202	0.0000	H	-2.3801	3.0686	0.0000
C	4.7551	-0.0341	0.0000	C	-4.9615	-1.0388	0.0000	H	-4.7199	2.3697	0.0000
C	4.9665	1.3168	0.0000	C	-3.6358	-1.3742	0.0000	H	-6.4247	0.5622	0.0000
C	3.8685	2.2076	-0.0000	H	-0.8603	-2.5856	0.8891	H	-5.7322	-1.8164	0.0000
C	2.5870	1.7293	0.0000	H	-0.8603	-2.5856	-0.8891	H	-3.3168	-2.4228	0.0000
C	-1.2575	-0.6448	0.0000	H	1.7971	-3.5779	0.0000				

Table 3.94: Table of thermodynamic data as a function of temperature for 1*H*-Dibenzo[*a,g*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-41.448	334.456	334.456	∞
100	92.978	330.529	684.564	-35.404	358.140	397.595	-207.678
200	176.718	419.143	529.853	-22.142	345.697	441.990	-115.434
250	226.339	463.855	512.164	-12.077	339.774	466.749	-97.520
298.15	275.256	507.908	507.908	0.000	334.456	491.698	-86.142
300	277.121	509.616	507.913	0.511	334.260	492.673	-85.780
350	326.304	556.062	511.469	15.608	329.323	519.476	-77.526
400	372.115	602.669	519.957	33.085	325.009	546.936	-71.421
450	413.731	648.943	531.723	52.749	321.258	574.905	-66.732
500	451.011	694.501	545.730	74.385	318.003	603.283	-63.023
600	513.721	782.496	577.922	122.744	312.721	660.862	-57.532
700	563.554	865.571	613.142	176.701	308.878	719.214	-53.667
800	603.734	943.539	649.621	235.134	306.300	778.014	-50.798
900	636.653	1016.611	686.382	297.206	304.819	837.067	-48.581
1000	663.977	1085.147	722.868	362.279	304.280	896.242	-46.814
1100	686.888	1149.536	758.759	429.855	304.509	955.441	-45.369
1200	706.251	1210.157	793.875	499.538	305.376	1014.575	-44.162
1300	722.724	1267.355	828.117	571.009	306.720	1073.626	-43.138
1400	736.819	1321.443	861.441	644.004	308.427	1132.562	-42.256
1500	748.946	1372.703	893.831	718.307	310.421	1191.367	-41.486
1600	759.430	1421.381	925.295	793.739	312.590	1250.025	-40.808
1700	768.540	1467.701	955.850	870.148	314.869	1308.524	-40.205
1800	776.490	1511.860	985.522	947.408	317.194	1366.939	-39.667
1900	783.461	1554.033	1014.342	1025.413	319.536	1425.182	-39.180
2000	789.598	1594.379	1042.343	1104.072	321.847	1483.323	-38.740
2100	795.024	1633.037	1069.557	1183.309	324.062	1541.339	-38.338
2200	799.840	1670.135	1096.019	1263.057	326.180	1599.256	-37.970
2300	804.130	1705.786	1121.760	1343.259	328.193	1657.075	-37.633
2400	807.966	1740.092	1146.814	1423.868	330.044	1714.774	-37.320
2500	811.408	1773.146	1171.210	1504.839	331.741	1772.489	-37.033
2600	814.506	1805.031	1194.978	1586.138	333.253	1830.047	-36.765
2700	817.303	1835.824	1218.146	1667.730	334.584	1887.604	-36.517
2800	819.835	1865.594	1240.741	1749.589	335.712	1945.137	-36.286
2900	822.136	1894.404	1262.787	1831.690	336.612	2002.590	-36.070
3000	824.230	1922.311	1284.308	1914.010	337.319	2060.035	-35.868
3100	826.142	1949.369	1305.328	1996.530	337.771	2117.402	-35.677
3200	827.892	1975.626	1325.866	2079.233	338.000	2174.815	-35.499
3300	829.497	2001.127	1345.944	2162.103	337.991	2232.253	-35.333
3400	830.973	2025.912	1365.580	2245.128	337.722	2289.631	-35.175
3500	832.332	2050.020	1384.793	2328.294	337.196	2347.005	-35.026
3600	833.587	2073.485	1403.599	2411.591	336.430	2404.464	-34.887
3700	834.747	2096.341	1422.014	2495.008	335.400	2461.965	-34.756
3800	835.823	2118.616	1440.054	2578.537	334.082	2519.445	-34.631
3900	836.821	2140.340	1457.733	2662.170	332.511	2576.928	-34.513
4000	837.750	2161.539	1475.064	2745.899	330.672	2634.561	-34.403
4100	838.614	2182.236	1492.061	2829.718	328.537	2692.185	-34.298
4200	839.421	2202.454	1508.735	2913.620	326.130	2749.857	-34.199
4300	840.174	2222.215	1525.099	2997.600	323.436	2807.520	-34.104
4400	840.879	2241.538	1541.163	3081.653	320.465	2865.322	-34.015
4500	841.539	2260.443	1556.937	3165.775	317.226	2923.240	-33.931
4600	842.159	2278.946	1572.433	3249.960	313.680	2981.236	-33.852
4700	842.741	2297.064	1587.658	3334.205	309.838	3039.223	-33.776
4800	843.288	2314.812	1602.623	3418.507	305.736	3097.378	-33.706
4900	843.803	2332.205	1617.336	3502.862	301.317	3155.516	-33.638
5000	844.289	2349.257	1631.804	3587.267	296.654	3213.897	-33.575

3.95. 7H-Indeno[1,2-a]phenanthrene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 198-08-3
Point Group: C_s

Length: 14.87 Å
Width: 9.192 Å
Breadth: 4.177 Å
L/B Ratio: 1.618

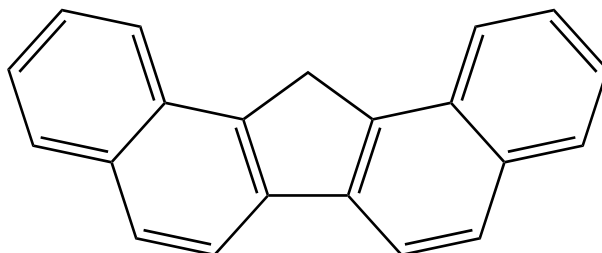
Cartesian coordinates:

C	2.7553	2.0861	0.0000	C	-1.2821	0.6962	0.0000	H	4.5293	-2.9535	0.0000
C	3.4161	0.7403	0.0000	C	-1.7052	-2.1028	0.0000	H	6.2215	-1.1465	0.0000
C	2.4399	-0.2874	0.0000	C	-0.4434	-1.6140	0.0000	H	5.5133	1.2471	0.0000
C	2.8409	-1.6149	0.0000	C	-2.8369	-1.2196	0.0000	H	0.3848	3.6944	0.0000
C	4.2055	-1.9074	0.0000	C	-2.6327	0.1709	0.0000	H	-1.9332	2.7591	0.0000
C	5.1562	-0.8938	0.0000	C	-3.7583	1.0232	0.0000	H	-1.8911	-3.1831	0.0000
C	4.7667	0.4470	0.0000	C	-5.0331	0.5048	0.0000	H	0.4151	-2.2994	0.0000
C	1.1127	0.3404	0.0000	C	-5.2316	-0.8855	0.0000	H	-3.5947	2.1115	0.0000
C	1.2967	1.7324	0.0000	C	-4.1500	-1.7366	0.0000	H	-5.9003	1.1732	0.0000
C	0.2167	2.6129	0.0000	H	3.0333	2.6824	0.8888	H	-6.2509	-1.2850	0.0000
C	-1.0599	2.0887	0.0000	H	3.0333	2.6824	-0.8888	H	-4.2967	-2.8227	0.0000
C	-0.1884	-0.2004	0.0000	H	2.1044	-2.4287	-0.0000				

Table 3.95: Table of thermodynamic data as a function of temperature for 7*H*-Indeno[1,2-*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.598	331.731	331.731	∞
100	93.442	336.151	690.285	-35.413	355.404	394.297	-205.955
200	176.728	424.923	535.581	-22.132	342.982	438.119	-114.422
250	226.222	469.622	517.901	-12.070	337.056	462.589	-96.651
298.15	275.072	513.648	513.648	0.000	331.731	487.261	-85.364
300	276.935	515.355	513.653	0.511	331.534	488.225	-85.006
350	326.093	561.770	517.206	15.597	326.587	514.742	-76.819
400	371.899	608.348	525.689	33.063	322.262	541.917	-70.766
450	413.521	654.597	537.448	52.717	318.501	569.603	-66.116
500	450.809	700.133	551.447	74.343	315.235	597.699	-62.440
600	513.530	788.092	583.621	122.683	309.933	654.717	-56.997
700	563.366	871.139	618.824	176.620	306.072	712.510	-53.167
800	603.547	949.081	655.288	235.035	303.475	770.755	-50.324
900	636.464	1022.131	692.033	297.088	301.975	829.255	-48.128
1000	663.790	1090.647	728.505	362.142	301.418	887.879	-46.377
1100	686.703	1155.019	764.383	429.699	301.628	946.528	-44.946
1200	706.071	1215.623	799.486	499.365	302.476	1005.115	-43.751
1300	722.551	1272.807	833.717	570.818	303.803	1063.620	-42.736
1400	736.655	1326.884	867.029	643.796	305.493	1122.012	-41.862
1500	748.789	1378.132	899.410	718.083	307.470	1180.273	-41.100
1600	759.283	1426.800	930.864	793.499	309.625	1238.389	-40.428
1700	768.400	1473.112	961.409	869.894	311.889	1296.346	-39.831
1800	776.359	1517.262	991.073	947.141	314.201	1354.220	-39.298
1900	783.337	1559.429	1019.885	1025.133	316.530	1411.924	-38.816
2000	789.482	1599.769	1047.878	1103.780	318.829	1469.526	-38.379
2100	794.915	1638.422	1075.086	1183.006	321.033	1527.003	-37.981
2200	799.737	1675.515	1101.541	1262.743	323.140	1584.381	-37.617
2300	804.034	1711.161	1127.276	1342.936	325.143	1641.663	-37.283
2400	807.876	1745.463	1152.324	1423.535	326.985	1698.825	-36.973
2500	811.323	1778.513	1176.714	1504.498	328.673	1756.003	-36.689
2600	814.425	1810.395	1200.477	1585.788	330.177	1813.024	-36.423
2700	817.227	1841.185	1223.640	1667.373	331.500	1870.045	-36.177
2800	819.764	1870.953	1246.230	1749.224	332.621	1927.042	-35.949
2900	822.068	1899.760	1268.271	1831.318	333.514	1983.959	-35.734
3000	824.166	1927.665	1289.788	1913.631	334.215	2040.868	-35.534
3100	826.082	1954.721	1310.804	1996.145	334.660	2097.700	-35.345
3200	827.835	1980.976	1331.338	2078.842	334.883	2154.578	-35.169
3300	829.443	2006.475	1351.413	2161.707	334.868	2211.482	-35.004
3400	830.921	2031.259	1371.045	2244.726	334.595	2268.325	-34.848
3500	832.283	2055.365	1390.255	2327.887	334.064	2325.164	-34.700
3600	833.540	2078.829	1409.057	2411.179	333.293	2382.088	-34.562
3700	834.703	2101.683	1427.469	2494.592	332.258	2439.055	-34.433
3800	835.780	2123.958	1445.506	2578.117	330.935	2496.001	-34.309
3900	836.781	2145.681	1463.182	2661.745	329.360	2552.950	-34.192
4000	837.711	2166.878	1480.510	2745.471	327.517	2610.049	-34.083
4100	838.577	2187.574	1497.504	2829.285	325.379	2667.139	-33.979
4200	839.385	2207.792	1514.176	2913.184	322.968	2724.277	-33.881
4300	840.140	2227.552	1530.538	2997.161	320.270	2781.407	-33.787
4400	840.846	2246.874	1546.599	3081.210	317.296	2838.675	-33.699
4500	841.508	2265.778	1562.372	3165.328	314.054	2896.060	-33.616
4600	842.129	2284.280	1577.865	3249.511	310.505	2953.521	-33.538
4700	842.712	2302.398	1593.088	3333.753	306.659	3010.976	-33.463
4800	843.260	2320.145	1608.051	3418.052	302.555	3068.597	-33.392
4900	843.776	2337.538	1622.762	3502.404	298.133	3126.202	-33.325
5000	844.263	2354.590	1637.228	3586.806	293.468	3184.050	-33.263

3.96. 1*H*-Dibenzo[*a,i*]fluorene



Other names: 1,2,7,8-Dibenzofluorene
 α,α' -Dinaphthofluorene

Formula: $C_{21}H_{14}$

Mass: 266.336 g/mol

CAS Number: 239-60-1

Point Group: C_{2v}

Length: 15.17 Å

Width: 8.712 Å

Breadth: 4.177 Å

L/B Ratio: 1.741

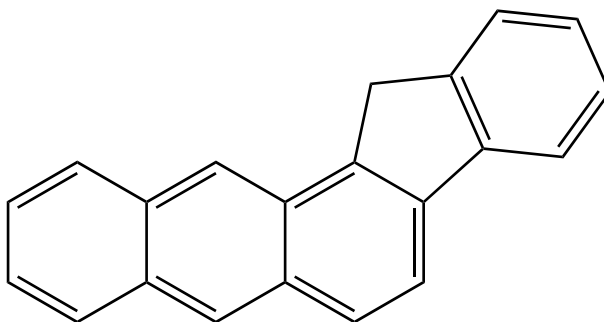
Cartesian coordinates:

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C	0.7300	1.1341	-0.0000	C	-1.6378	2.2094	0.0000	H	2.3359	-2.6465	-0.0000
C	1.1730	-0.1877	-0.0000	C	-2.9821	1.9352	0.0000	H	4.7909	-3.0698	0.0000
C	2.9804	1.9378	0.0000	C	-2.5525	-0.4890	-0.0000	H	6.3859	-1.1741	0.0000
C	1.6359	2.2108	0.0000	C	-3.4609	0.5960	0.0000	H	5.5587	1.1677	0.0000
C	3.4604	0.5990	0.0000	C	-4.8566	0.3222	0.0000	H	-1.2613	3.2376	0.0000
C	2.5529	-0.4867	-0.0000	C	-5.3106	-0.9683	0.0000	H	-3.7127	2.7523	0.0000
C	3.0523	-1.8172	0.0000	C	-4.3987	-2.0507	0.0000	H	-5.5597	1.1629	0.0000
C	4.4005	-2.0469	0.0000	C	-3.0508	-1.8198	0.0000	H	-6.3849	-1.1796	0.0000
C	5.3114	-0.9637	0.0000	H	0.0008	-1.7876	0.8891	H	-4.7882	-3.0739	0.0000
C	4.8563	0.3264	0.0000	H	0.0008	-1.7876	-0.8891	H	-2.3337	-2.6486	-0.0000
C	-1.1728	-0.1887	-0.0000	H	3.7103	2.7555	0.0000				

Table 3.96: Table of thermodynamic data as a function of temperature for 1*H*-Dibenzo[*a,i*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-41.254	324.287	324.287	∞
100	92.468	320.946	674.184	-35.324	348.050	388.464	-202.908
200	176.318	409.272	519.789	-22.103	335.567	433.834	-113.303
250	225.944	453.895	502.129	-12.059	329.624	459.088	-95.919
298.15	274.880	497.879	497.879	0.000	324.287	484.519	-84.884
300	276.746	499.585	497.884	0.510	324.090	485.512	-84.533
350	325.956	545.975	501.436	15.589	319.135	512.819	-76.532
400	371.794	592.537	509.914	33.049	314.804	540.783	-70.618
450	413.440	638.775	521.668	52.698	311.038	569.261	-66.077
500	450.753	684.304	535.663	74.321	307.769	598.147	-62.487
600	513.533	772.258	567.829	122.657	302.464	656.749	-57.174
700	563.437	855.310	603.027	176.599	298.607	716.125	-53.437
800	603.683	933.266	639.487	235.024	296.020	775.952	-50.663
900	636.656	1006.336	676.232	297.094	294.537	836.032	-48.521
1000	664.022	1074.874	712.705	362.169	294.001	896.236	-46.814
1100	686.962	1139.269	748.587	429.751	294.236	956.461	-45.418
1200	706.346	1199.897	783.695	499.443	295.111	1016.621	-44.251
1300	722.832	1257.103	817.932	570.923	296.466	1076.698	-43.261
1400	736.935	1311.201	851.251	643.930	298.184	1136.659	-42.408
1500	749.065	1362.468	883.638	718.245	300.189	1196.487	-41.665
1600	759.551	1411.154	915.099	793.688	302.370	1256.168	-41.009
1700	768.658	1457.481	945.652	870.109	304.661	1315.690	-40.425
1800	776.606	1501.647	975.324	947.381	306.998	1375.126	-39.904
1900	783.573	1543.826	1004.143	1025.398	309.352	1434.391	-39.433
2000	789.706	1584.177	1032.143	1104.068	311.673	1493.552	-39.007
2100	795.127	1622.841	1059.358	1183.315	313.899	1552.588	-38.618
2200	799.939	1659.944	1085.820	1263.073	316.027	1611.524	-38.262
2300	804.225	1695.599	1111.562	1343.285	318.049	1670.362	-37.934
2400	808.056	1729.909	1136.616	1423.903	319.910	1729.080	-37.632
2500	811.493	1762.966	1161.013	1504.884	321.616	1787.813	-37.354
2600	814.587	1794.855	1184.782	1586.190	323.136	1846.388	-37.094
2700	817.380	1825.651	1207.951	1667.791	324.475	1904.963	-36.853
2800	819.909	1855.424	1230.546	1749.657	325.611	1963.514	-36.629
2900	822.206	1884.236	1252.593	1831.765	326.518	2021.983	-36.419
3000	824.297	1912.146	1274.115	1914.092	327.232	2080.444	-36.223
3100	826.206	1939.206	1295.135	1996.618	327.690	2138.828	-36.038
3200	827.953	1965.465	1315.675	2079.328	327.926	2197.257	-35.866
3300	829.555	1990.967	1335.754	2162.204	327.922	2255.712	-35.704
3400	831.028	2015.754	1355.391	2245.234	327.659	2314.106	-35.551
3500	832.385	2039.863	1374.605	2328.406	327.139	2372.496	-35.407
3600	833.637	2063.330	1393.411	2411.708	326.378	2430.970	-35.272
3700	834.795	2086.187	1411.827	2495.130	325.352	2489.486	-35.145
3800	835.869	2108.464	1429.868	2578.664	324.039	2547.982	-35.024
3900	836.865	2130.189	1447.548	2662.301	322.472	2606.480	-34.909
4000	837.792	2151.388	1464.880	2746.035	320.638	2665.128	-34.802
4100	838.655	2172.086	1481.877	2829.857	318.508	2723.766	-34.700
4200	839.459	2192.306	1498.553	2913.764	316.104	2782.454	-34.604
4300	840.211	2212.068	1514.917	2997.748	313.414	2841.132	-34.512
4400	840.915	2231.392	1530.982	3081.804	310.446	2899.949	-34.426
4500	841.574	2250.297	1546.757	3165.929	307.211	2958.881	-34.345
4600	842.192	2268.801	1562.253	3250.118	303.669	3017.891	-34.269
4700	842.773	2286.919	1577.480	3334.366	299.829	3076.893	-34.195
4800	843.319	2304.668	1592.445	3418.671	295.731	3136.062	-34.127
4900	843.833	2322.062	1607.158	3503.029	291.315	3195.215	-34.061
5000	844.317	2339.115	1621.628	3587.437	286.655	3254.610	-34.000

3.97. 1*H*-Indeno[2,1-*a*]anthracene



Other names: 1*H*-Naphtho[2,3-*a*]fluorene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 223-31-4

Point Group: C_s

Length: 15.54 Å

Width: 8.753 Å

Breadth: 4.177 Å

L/B Ratio: 1.775

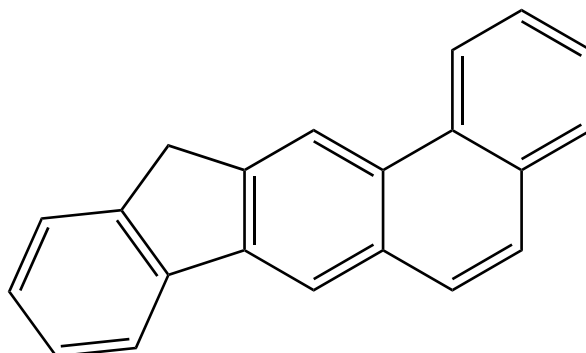
Cartesian coordinates:

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C	5.6026	-0.3683	-0.0000	C	-1.7050	0.9079	0.0000	H	2.8220	2.5770	0.0000
C	4.7466	0.6883	-0.0000	C	-1.6330	-1.4686	0.0000	H	1.0671	-2.1075	0.0000
C	3.7666	-1.9435	-0.0000	C	-3.0565	-0.9866	0.0000	H	0.5519	3.4483	0.0000
C	2.8328	-0.8558	0.0000	C	-3.0855	0.4289	0.0000	H	-1.9185	3.0719	-0.0000
C	3.3288	0.4769	0.0000	C	-4.2886	1.1150	-0.0000	H	-1.4067	-2.0862	0.8889
C	2.4357	1.5501	0.0000	C	-5.4702	0.3722	-0.0000	H	-1.4067	-2.0862	-0.8889
C	1.4556	-1.0815	0.0000	C	-5.4423	-1.0186	-0.0000	H	-4.3085	2.2095	-0.0000
C	0.5613	-0.0078	0.0000	C	-4.2314	-1.7150	0.0000	H	-6.4330	0.8938	-0.0000
C	1.0550	1.3301	0.0000	H	5.8225	-2.5313	-0.0000	H	-6.3833	-1.5784	-0.0000
C	0.1378	2.4333	0.0000	H	6.6863	-0.2119	-0.0000	H	-4.2144	-2.8090	0.0000
C	-1.2111	2.2361	0.0000	H	5.1201	1.7186	-0.0000				

Table 3.97: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[2,1-*a*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.334	336.819	336.819	∞
100	92.496	327.487	681.339	-35.385	360.521	400.280	-209.081
200	176.645	415.936	526.662	-22.145	348.057	444.991	-116.217
250	226.377	460.644	508.969	-12.081	342.133	469.910	-98.180
298.15	275.383	504.712	504.712	0.000	336.819	495.014	-86.723
300	277.250	506.421	504.717	0.511	336.623	495.995	-86.359
350	326.485	552.891	508.274	15.616	331.694	522.957	-78.045
400	372.314	599.523	516.767	33.102	327.390	550.574	-71.896
450	413.932	645.821	528.539	52.777	323.649	578.701	-67.172
500	451.207	691.400	542.554	74.423	320.403	607.234	-63.436
600	513.913	779.430	574.761	122.801	315.141	665.122	-57.903
700	563.756	862.536	609.997	176.777	311.318	723.778	-54.008
800	603.955	940.531	646.491	235.232	308.760	782.881	-51.116
900	636.892	1013.631	683.267	297.327	307.302	842.233	-48.881
1000	664.230	1082.192	719.768	362.424	306.789	901.705	-47.099
1100	687.148	1146.606	755.674	430.026	307.043	961.198	-45.643
1200	706.512	1207.249	790.803	499.736	307.936	1020.624	-44.426
1300	722.982	1264.468	825.059	571.232	309.306	1079.964	-43.393
1400	737.072	1318.576	858.395	644.253	311.039	1139.188	-42.503
1500	749.189	1369.852	890.798	718.581	313.057	1198.279	-41.727
1600	759.664	1418.546	922.274	794.036	315.250	1257.221	-41.043
1700	768.762	1464.880	952.840	870.468	317.552	1316.003	-40.435
1800	776.702	1509.051	982.523	947.750	319.899	1374.699	-39.892
1900	783.661	1551.236	1011.354	1025.775	322.262	1433.223	-39.401
2000	789.787	1591.591	1039.364	1104.454	324.592	1491.643	-38.957
2100	795.203	1630.259	1066.588	1183.709	326.825	1549.937	-38.552
2200	800.008	1667.365	1093.058	1263.474	328.961	1608.132	-38.181
2300	804.289	1703.023	1118.808	1343.693	330.990	1666.228	-37.840
2400	808.117	1737.335	1143.870	1424.317	332.856	1724.203	-37.526
2500	811.550	1770.395	1168.274	1505.304	334.568	1782.193	-37.236
2600	814.640	1802.286	1192.049	1586.616	336.094	1840.025	-36.966
2700	817.430	1833.084	1215.224	1668.222	337.438	1897.857	-36.715
2800	819.956	1862.858	1237.825	1750.093	338.578	1955.664	-36.483
2900	822.249	1891.672	1259.877	1832.205	339.490	2013.390	-36.264
3000	824.338	1919.584	1281.405	1914.536	340.208	2071.108	-36.060
3100	826.245	1946.645	1302.430	1997.066	340.671	2128.748	-35.868
3200	827.989	1972.905	1322.974	2079.779	340.910	2186.433	-35.689
3300	829.589	1998.409	1343.057	2162.660	340.910	2244.143	-35.521
3400	831.061	2023.196	1362.698	2245.693	340.650	2301.793	-35.362
3500	832.416	2047.307	1381.916	2328.868	340.133	2359.438	-35.212
3600	833.667	2070.774	1400.726	2412.173	339.375	2417.168	-35.071
3700	834.824	2093.632	1419.146	2495.598	338.352	2474.940	-34.939
3800	835.896	2115.910	1437.190	2579.135	337.042	2532.691	-34.814
3900	836.891	2137.635	1454.873	2662.775	335.478	2590.445	-34.694
4000	837.816	2158.835	1472.208	2746.510	333.646	2648.348	-34.583
4100	838.678	2179.534	1489.208	2830.336	331.518	2706.242	-34.477
4200	839.482	2199.754	1505.886	2914.244	329.116	2764.185	-34.377
4300	840.233	2219.516	1522.253	2998.230	326.428	2822.118	-34.281
4400	840.935	2238.841	1538.321	3082.289	323.463	2880.189	-34.191
4500	841.593	2257.746	1554.099	3166.416	320.230	2938.377	-34.107
4600	842.211	2276.251	1569.597	3250.606	316.689	2996.642	-34.027
4700	842.791	2294.370	1584.826	3334.857	312.852	3054.899	-33.951
4800	843.336	2312.119	1599.793	3419.163	308.755	3113.323	-33.879
4900	843.849	2329.513	1614.509	3503.523	304.341	3171.731	-33.810
5000	844.333	2346.566	1628.980	3587.932	299.682	3230.381	-33.747

3.98. 1*H*-Indeno[1,2-*b*]phenanthrene



Other names: 1',2'-Naphtha-2,3-fluorene
12H-Naphtho[1,2-*b*]fluorene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 248-83-9

Point Group: C_s

Length: 15.64 Å

Width: 8.479 Å

Breadth: 4.176 Å

L/B Ratio: 1.845

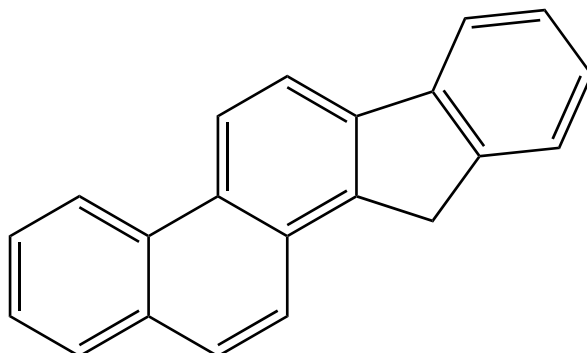
Cartesian coordinates:

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C	2.9598	0.4129	0.0000	C	-1.7204	2.2772	0.0000	H	5.9767	1.9378	0.0000
C	3.3898	-0.9353	0.0000	C	-3.0531	2.0347	0.0000	H	3.5405	2.4928	0.0000
C	4.7371	-1.2430	0.0000	C	-2.6538	-0.3906	0.0000	H	0.9676	2.5183	0.0000
C	5.6589	-0.1922	0.0000	C	-3.5538	0.6898	0.0000	H	-0.6753	-2.2369	0.0000
C	5.2357	1.1317	0.0000	C	-4.9440	0.4408	0.0000	H	-1.3356	3.3036	0.0000
C	3.8759	1.4508	0.0000	C	-5.4187	-0.8503	0.0000	H	-3.7765	2.8582	0.0000
C	1.0381	-0.9197	0.0000	C	-4.5219	-1.9325	0.0000	H	-5.6381	1.2889	0.0000
C	1.4988	0.4323	0.0000	C	-3.1653	-1.7073	0.0000	H	-6.4963	-1.0440	0.0000
C	0.6153	1.4806	0.0000	H	2.2039	-2.5218	0.8885	H	-4.9120	-2.9555	0.0000
C	-0.3004	-1.2026	0.0000	H	2.2039	-2.5218	-0.8885	H	-2.4517	-2.5455	0.0000
C	-1.2313	-0.1327	0.0000	H	5.0755	-2.2836	0.0000				

Table 3.98: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[1,2-*b*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.360	316.996	316.996	∞
100	92.771	328.953	682.543	-35.359	340.724	380.337	-198.663
200	176.450	417.409	528.012	-22.121	328.258	424.898	-110.970
250	226.117	462.065	510.338	-12.068	322.323	449.745	-93.967
298.15	275.120	506.085	506.085	0.000	316.996	474.781	-83.178
300	276.988	507.793	506.090	0.511	316.800	475.760	-82.835
350	326.254	554.225	509.645	15.603	311.858	502.654	-75.015
400	372.122	600.828	518.131	33.079	307.543	530.206	-69.236
450	413.774	647.106	529.896	52.745	303.794	558.267	-64.801
500	451.077	692.669	543.902	74.384	300.541	586.736	-61.295
600	513.811	780.679	576.095	122.751	295.267	644.498	-56.107
700	563.661	863.770	611.317	176.717	291.434	703.031	-52.460
800	603.858	941.753	647.800	235.162	288.867	762.011	-49.753
900	636.791	1014.840	684.566	297.247	287.399	821.241	-47.663
1000	664.125	1083.391	721.057	362.334	286.875	880.593	-45.997
1100	687.042	1147.795	756.954	429.925	287.119	939.966	-44.634
1200	706.407	1208.429	792.075	499.624	288.001	999.274	-43.496
1300	722.879	1265.639	826.324	571.110	289.361	1058.497	-42.530
1400	736.972	1319.739	859.653	644.121	291.084	1117.604	-41.697
1500	749.093	1371.009	892.050	718.439	293.092	1176.579	-40.971
1600	759.572	1419.697	923.519	793.885	295.276	1235.406	-40.331
1700	768.675	1466.025	954.079	870.308	297.569	1294.073	-39.761
1800	776.619	1510.191	983.757	947.581	299.907	1352.655	-39.252
1900	783.583	1552.372	1012.583	1025.599	302.262	1411.065	-38.792
2000	789.714	1592.723	1040.588	1104.270	304.584	1469.372	-38.375
2100	795.133	1631.387	1067.807	1183.518	306.811	1527.553	-37.995
2200	799.943	1668.490	1094.274	1263.276	308.939	1585.634	-37.647
2300	804.228	1704.145	1120.020	1343.489	310.962	1643.618	-37.327
2400	808.059	1738.455	1145.078	1424.107	312.823	1701.481	-37.031
2500	811.495	1771.513	1169.478	1505.088	314.529	1759.359	-36.759
2600	814.588	1803.402	1193.250	1586.394	316.050	1817.080	-36.505
2700	817.381	1834.198	1216.422	1667.995	317.388	1874.800	-36.269
2800	819.910	1863.970	1239.020	1749.862	318.524	1932.496	-36.050
2900	822.206	1892.783	1261.069	1831.969	319.431	1990.110	-35.845
3000	824.297	1920.693	1282.594	1914.296	320.145	2047.717	-35.653
3100	826.205	1947.753	1303.616	1996.823	320.604	2105.247	-35.472
3200	827.952	1974.012	1324.158	2079.532	320.839	2162.821	-35.304
3300	829.554	1999.514	1344.239	2162.408	320.835	2220.421	-35.146
3400	831.027	2024.301	1363.878	2245.438	320.572	2277.960	-34.996
3500	832.384	2048.410	1383.093	2328.610	320.052	2335.495	-34.855
3600	833.636	2071.877	1401.901	2411.912	319.291	2393.114	-34.722
3700	834.795	2094.734	1420.319	2495.334	318.265	2450.776	-34.598
3800	835.868	2117.011	1438.361	2578.868	316.952	2508.417	-34.480
3900	836.864	2138.736	1456.042	2662.505	315.385	2566.061	-34.368
4000	837.791	2159.935	1473.376	2746.238	313.550	2623.854	-34.263
4100	838.653	2180.633	1490.374	2830.061	311.420	2681.638	-34.164
4200	839.458	2200.852	1507.051	2913.967	309.016	2739.471	-34.070
4300	840.210	2220.614	1523.416	2997.951	306.326	2797.294	-33.980
4400	840.914	2239.938	1539.482	3082.007	303.358	2855.256	-33.895
4500	841.573	2258.843	1555.259	3166.132	300.123	2913.334	-33.816
4600	842.191	2277.347	1570.756	3250.321	296.581	2971.489	-33.742
4700	842.772	2295.466	1585.983	3334.569	292.741	3029.637	-33.670
4800	843.318	2313.215	1600.949	3418.874	288.643	3087.951	-33.603
4900	843.832	2330.609	1615.664	3503.231	284.227	3146.249	-33.539
5000	844.317	2347.661	1630.134	3587.639	279.566	3204.789	-33.480

3.99. 1*H*-Indeno[2,1-*a*]phenanthrene



Other names: 2',1'-Naphtha-1,2-fluorene
11*H*-Naphtho[2,1-*a*]fluorene

Formula: C₂₁H₁₄
Mass: 266.336 g/mol

CAS Number: 220-97-3

Point Group: C_s

Length: 15.51 Å

Width: 7.962 Å

Breadth: 4.176 Å

L/B Ratio: 1.948

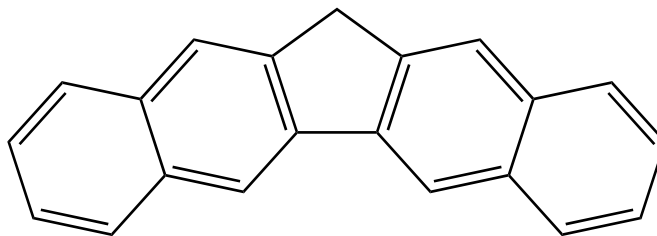
Cartesian coordinates:

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C	3.2444	-0.7989	0.0000	C	-1.1110	-1.9791	0.0000	H	3.7250	2.5993	0.0000
C	4.5557	-1.2360	0.0000	C	-3.2997	-0.9317	0.0000	H	1.1809	2.8799	0.0000
C	5.5737	-0.2790	0.0000	C	-2.7209	0.3499	0.0000	H	-1.3143	2.6431	0.0000
C	5.2801	1.0803	0.0000	C	-3.5650	1.4809	0.0000	H	-2.9393	-3.0827	0.0000
C	3.9584	1.5298	0.0000	C	-4.9336	1.3356	0.0000	H	-0.4626	-2.8630	0.0000
C	0.9091	-0.5371	0.0000	C	-5.5082	0.0543	0.0000	H	-3.1025	2.4798	0.0000
C	1.4932	0.7370	0.0000	C	-4.7046	-1.0636	0.0000	H	-5.5821	2.2178	0.0000
C	0.7080	1.8924	0.0000	H	1.9000	-2.2547	0.8888	H	-6.5982	-0.0481	-0.0000
C	-0.6655	1.7535	0.0000	H	1.9000	-2.2547	-0.8888	H	-5.1475	-2.0661	0.0000
C	-0.4856	-0.6859	0.0000	H	4.7917	-2.3044	0.0000				

Table 3.99: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[2,1-*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.072	319.593	319.593	∞
100	92.060	326.738	678.158	-35.142	343.538	383.372	-200.249
200	175.361	414.606	524.559	-21.991	330.985	428.185	-111.828
250	224.779	458.992	506.989	-11.999	324.989	453.179	-94.685
298.15	273.589	502.759	502.759	0.000	319.593	478.370	-83.807
300	275.452	504.458	502.765	0.508	319.394	479.354	-83.461
350	324.603	550.643	506.300	15.520	314.372	506.422	-75.578
400	370.436	597.023	514.742	32.912	309.973	534.158	-69.752
450	412.112	643.103	526.449	52.494	306.140	562.415	-65.282
500	449.475	688.494	540.391	74.051	302.805	591.089	-61.749
600	512.381	776.226	572.449	122.266	297.379	649.283	-56.524
700	562.411	859.110	607.540	176.099	293.413	708.271	-52.851
800	602.769	936.937	643.903	234.427	290.729	767.725	-50.126
900	635.839	1009.904	680.560	296.410	289.159	827.444	-48.023
1000	663.289	1078.361	716.953	361.408	288.546	887.294	-46.347
1100	686.302	1142.690	752.762	428.921	288.712	947.174	-44.977
1200	705.750	1203.263	787.805	498.550	289.524	1006.996	-43.832
1300	722.292	1260.424	821.982	569.974	290.822	1066.738	-42.861
1400	736.445	1314.483	855.248	642.929	292.489	1126.368	-42.024
1500	748.618	1365.718	887.586	717.197	294.447	1185.870	-41.295
1600	759.142	1414.376	919.003	792.598	296.586	1245.228	-40.652
1700	768.284	1460.680	949.515	868.979	298.837	1304.428	-40.079
1800	776.263	1504.825	979.149	946.216	301.139	1363.546	-39.568
1900	783.257	1546.986	1007.934	1024.199	303.459	1422.494	-39.106
2000	789.414	1587.322	1035.903	1102.839	305.750	1481.340	-38.688
2100	794.858	1625.972	1063.087	1182.058	307.948	1540.062	-38.306
2200	799.688	1663.063	1089.522	1261.790	310.050	1598.685	-37.957
2300	803.992	1698.707	1115.238	1341.978	312.048	1657.212	-37.636
2400	807.840	1733.007	1140.268	1422.573	313.886	1715.620	-37.339
2500	811.292	1766.056	1164.643	1503.533	315.571	1774.043	-37.066
2600	814.398	1797.937	1188.391	1584.820	317.072	1832.310	-36.811
2700	817.203	1828.726	1211.540	1666.403	318.393	1890.577	-36.575
2800	819.743	1858.493	1234.117	1748.252	319.511	1948.820	-36.355
2900	822.050	1887.300	1256.147	1830.344	320.403	2006.983	-36.149
3000	824.150	1915.204	1277.653	1912.655	321.101	2065.138	-35.957
3100	826.068	1942.260	1298.657	1995.168	321.546	2123.217	-35.775
3200	827.822	1968.514	1319.182	2077.863	321.767	2181.340	-35.606
3300	829.431	1994.013	1339.247	2160.727	321.751	2239.490	-35.447
3400	830.911	2018.796	1358.871	2243.745	321.476	2297.579	-35.297
3500	832.274	2042.902	1378.072	2326.905	320.944	2355.665	-35.156
3600	833.532	2066.366	1396.867	2410.197	320.173	2413.836	-35.023
3700	834.695	2089.220	1415.272	2493.609	319.137	2472.049	-34.898
3800	835.774	2111.494	1433.301	2577.133	317.814	2530.241	-34.780
3900	836.775	2133.217	1450.971	2660.761	316.238	2588.436	-34.668
4000	837.705	2154.414	1468.293	2744.485	314.394	2646.782	-34.563
4100	838.572	2175.110	1485.281	2828.300	312.256	2705.118	-34.463
4200	839.380	2195.327	1501.947	2912.198	309.844	2763.503	-34.368
4300	840.136	2215.087	1518.303	2996.174	307.146	2821.879	-34.278
4400	840.842	2234.410	1534.359	3080.223	304.171	2880.394	-34.194
4500	841.504	2253.314	1550.127	3164.341	300.929	2939.025	-34.115
4600	842.126	2271.816	1565.615	3248.523	297.380	2997.733	-34.040
4700	842.709	2289.933	1580.834	3332.765	293.534	3056.434	-33.968
4800	843.257	2307.681	1595.792	3417.063	289.429	3115.301	-33.901
4900	843.774	2325.073	1610.499	3501.415	285.007	3174.153	-33.836
5000	844.261	2342.125	1624.961	3585.817	280.341	3233.247	-33.777

3.100. 1*H*-Dibenzo[*b,h*]fluorene



Other names: Di- β -naphthofluorene
2,3,6,7-Dibenzofluorene

Formula: C₂₁H₁₄
Mass: 266.336 g/mol

CAS Number: 242-47-7

Point Group: C_{2v}

Length: 16.06 Å
Width: 8.268 Å
Breadth: 4.176 Å
L/B Ratio: 1.942

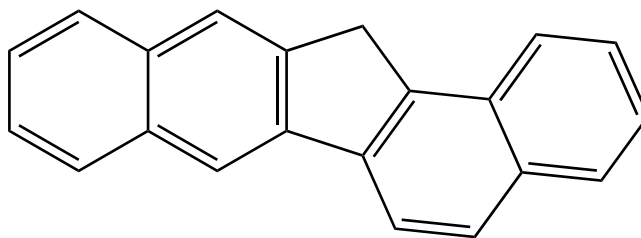
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C	-3.9726	-1.8291	0.0000	C	2.5068	1.6252	0.0000	H	-2.8597	2.6624	0.0000
C	-4.8473	0.8284	0.0000	C	3.4543	0.5573	0.0000	H	0.0003	2.9149	0.8882
C	-3.4541	0.5580	0.0000	C	3.0125	-0.7841	0.0000	H	0.0003	2.9149	-0.8882
C	-3.0126	-0.7834	0.0000	C	3.9722	-1.8299	0.0000	H	1.2779	-2.1202	0.0000
C	-1.6171	-1.0778	0.0000	C	5.3115	-1.5419	0.0000	H	2.8602	2.6618	0.0000
C	-2.5065	1.6257	0.0000	C	5.7533	-0.2005	0.0000	H	3.6231	-2.8687	0.0000
C	-1.1786	1.3245	0.0000	C	4.8475	0.8274	0.0000	H	6.0529	-2.3475	0.0000
C	-0.7304	-0.0409	0.0000	H	-6.8283	0.0082	0.0000	H	6.8284	0.0068	0.0000
C	0.0002	2.2561	0.0000	H	-6.0534	-2.3462	0.0000	H	5.1847	1.8701	0.0000
C	1.1789	1.3242	0.0000	H	-3.6237	-2.8679	0.0000				

Table 3.100: Table of thermodynamic data as a function of temperature for 1*H*-Dibenzo[*b,h*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-41.328	319.158	319.158	∞
100	92.006	322.437	676.218	-35.378	342.867	383.131	-200.123
200	176.625	410.689	521.508	-22.164	330.377	428.361	-111.874
250	226.576	455.417	503.797	-12.095	324.458	453.542	-94.760
298.15	275.753	499.534	499.534	0.000	319.158	478.896	-83.899
300	277.625	501.246	499.540	0.512	318.963	479.887	-83.554
350	326.972	547.783	503.102	15.638	314.055	507.106	-75.680
400	372.854	594.484	511.607	33.151	309.777	534.977	-69.859
450	414.482	640.847	523.397	52.852	306.063	563.354	-65.391
500	451.743	686.483	537.431	74.526	302.845	592.134	-61.859
600	514.389	774.606	569.681	122.955	297.633	650.509	-56.631
700	564.167	857.780	604.958	176.975	293.854	709.644	-52.953
800	604.311	935.827	641.492	235.468	291.335	769.219	-50.224
900	637.202	1008.965	678.303	297.597	289.910	829.040	-48.115
1000	664.503	1077.558	714.835	362.723	289.426	888.977	-46.434
1100	687.391	1141.996	750.769	430.350	289.706	948.932	-45.060
1200	706.730	1202.659	785.924	500.083	290.622	1008.818	-43.912
1300	723.179	1259.895	820.202	571.600	292.013	1068.616	-42.937
1400	737.250	1314.017	853.560	644.640	293.765	1128.297	-42.096
1500	749.351	1365.305	885.981	718.985	295.800	1187.843	-41.364
1600	759.812	1414.009	917.474	794.455	298.008	1247.239	-40.717
1700	768.897	1460.351	948.056	870.901	300.324	1306.475	-40.142
1800	776.826	1504.529	977.754	948.196	302.684	1365.623	-39.629
1900	783.775	1546.720	1006.597	1026.234	305.059	1424.599	-39.164
2000	789.893	1587.082	1034.620	1104.924	307.400	1483.470	-38.743
2100	795.300	1625.754	1061.855	1184.189	309.644	1542.215	-38.360
2200	800.099	1662.864	1088.336	1263.963	311.788	1600.860	-38.008
2300	804.373	1698.526	1114.095	1344.191	313.826	1659.406	-37.686
2400	808.195	1732.842	1139.166	1424.823	315.701	1717.831	-37.387
2500	811.623	1765.905	1163.578	1505.817	317.420	1776.269	-37.112
2600	814.708	1797.799	1187.362	1587.136	318.953	1834.551	-36.856
2700	817.494	1828.599	1210.544	1668.749	320.304	1892.831	-36.618
2800	820.016	1858.376	1233.152	1750.626	321.450	1951.087	-36.397
2900	822.306	1887.192	1255.211	1832.744	322.368	2009.260	-36.190
3000	824.391	1915.105	1276.745	1915.081	323.091	2067.426	-35.996
3100	826.295	1942.168	1297.776	1997.616	323.559	2125.514	-35.814
3200	828.037	1968.430	1318.325	2080.334	323.803	2183.647	-35.644
3300	829.634	1993.935	1338.414	2163.219	323.808	2241.805	-35.484
3400	831.103	2018.724	1358.060	2246.257	323.553	2299.901	-35.333
3500	832.456	2042.835	1377.282	2329.436	323.039	2357.994	-35.190
3600	833.705	2066.304	1396.097	2412.744	322.285	2416.171	-35.057
3700	834.860	2089.163	1414.521	2496.173	321.266	2474.390	-34.931
3800	835.930	2111.441	1432.569	2579.714	319.959	2532.588	-34.812
3900	836.924	2133.168	1450.256	2663.357	318.399	2590.788	-34.699
4000	837.847	2154.369	1467.595	2747.096	316.570	2649.138	-34.593
4100	838.708	2175.068	1484.599	2830.924	314.445	2707.479	-34.493
4200	839.510	2195.289	1501.280	2914.836	312.046	2765.868	-34.398
4300	840.260	2215.052	1517.651	2998.825	309.361	2824.248	-34.307
4400	840.961	2234.377	1533.721	3082.886	306.399	2882.766	-34.222
4500	841.618	2253.283	1549.502	3167.015	303.168	2941.400	-34.142
4600	842.235	2271.788	1565.004	3251.208	299.630	3000.111	-34.067
4700	842.814	2289.908	1580.235	3335.461	295.795	3058.814	-33.994
4800	843.358	2307.657	1595.205	3419.770	291.701	3117.685	-33.927
4900	843.871	2325.052	1609.923	3504.132	287.289	3176.538	-33.862
5000	844.354	2342.106	1624.397	3588.543	282.632	3235.634	-33.802

3.101. 1*H*-Dibenzo[*a,h*]fluorene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 239-85-0
Point Group: C_s

Length: 15.80 Å
Width: 7.963 Å
Breadth: 4.176 Å
L/B Ratio: 1.984

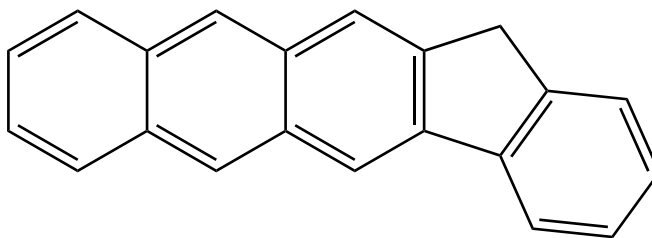
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C	1.8048	1.2987	0.0000	C	-3.4875	0.7548	0.0000	H	4.1271	2.6524	0.0000
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C	4.5906	-1.2135	0.0000	C	-4.9330	-1.6524	0.0000	H	-5.4317	1.7281	0.0000
C	5.6828	-0.3869	0.0000	C	-3.5664	-1.6944	0.0000	H	-6.7065	-0.4037	0.0000
C	5.5170	1.0159	0.0000	H	-0.5906	-2.2796	0.8885	H	-5.5185	-2.5776	0.0000
C	4.2622	1.5649	0.0000	H	-0.5906	-2.2796	-0.8885	H	-3.0287	-2.6495	0.0000
C	-1.4006	-0.4710	-0.0000	H	2.2784	-2.6163	0.0000				

Table 3.101: Table of thermodynamic data as a function of temperature for 1*H*-Dibenzo[*a,h*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-41.074	320.578	320.578	∞
100	91.585	325.817	677.775	-35.196	344.469	384.395	-200.783
200	175.679	413.617	523.866	-22.050	331.911	429.309	-112.122
250	225.400	458.108	506.246	-12.034	325.938	454.350	-94.929
298.15	274.423	502.004	502.004	0.000	320.578	479.580	-84.019
300	276.292	503.707	502.009	0.509	320.380	480.566	-83.672
350	325.568	550.033	505.556	15.567	315.404	507.667	-75.764
400	371.453	596.546	514.023	33.009	311.055	535.431	-69.919
450	413.132	642.746	525.764	52.642	307.273	563.708	-65.432
500	450.470	688.244	539.744	74.250	303.989	592.397	-61.886
600	513.291	776.150	571.883	122.560	298.658	650.607	-56.639
700	563.233	859.168	607.055	176.479	294.778	709.596	-52.950
800	603.514	937.099	643.492	234.886	292.173	769.039	-50.212
900	636.517	1010.150	680.217	296.940	290.674	828.737	-48.098
1000	663.909	1078.675	716.673	362.003	290.126	888.559	-46.413
1100	686.871	1143.061	752.538	429.575	290.350	948.405	-45.035
1200	706.272	1203.681	787.633	499.258	291.217	1008.187	-43.884
1300	722.772	1260.882	821.857	570.733	292.565	1067.885	-42.907
1400	736.887	1314.975	855.166	643.734	294.278	1127.468	-42.065
1500	749.025	1366.240	887.544	718.044	296.279	1186.919	-41.331
1600	759.518	1414.924	918.996	793.484	298.457	1246.224	-40.684
1700	768.631	1461.249	949.542	869.902	300.745	1305.368	-40.108
1800	776.583	1505.413	979.207	947.171	303.079	1364.428	-39.594
1900	783.554	1547.591	1008.020	1025.186	305.430	1423.316	-39.129
2000	789.690	1587.942	1036.015	1103.854	307.750	1482.101	-38.708
2100	795.114	1626.605	1063.224	1183.100	309.975	1540.760	-38.324
2200	799.927	1663.707	1089.681	1262.857	312.101	1599.320	-37.972
2300	804.214	1699.361	1115.419	1343.068	314.123	1657.782	-37.649
2400	808.047	1733.671	1140.469	1423.684	315.982	1716.123	-37.350
2500	811.486	1766.728	1164.862	1504.664	317.687	1774.480	-37.075
2600	814.580	1798.616	1188.628	1585.970	319.207	1832.679	-36.818
2700	817.374	1829.412	1211.793	1667.570	320.545	1890.878	-36.580
2800	819.904	1859.185	1234.386	1749.436	321.680	1949.053	-36.359
2900	822.201	1887.997	1256.430	1831.543	322.587	2007.146	-36.152
3000	824.293	1915.906	1277.950	1913.870	323.300	2065.231	-35.958
3100	826.202	1942.966	1298.968	1996.396	323.759	2123.239	-35.776
3200	827.949	1969.225	1319.505	2079.105	323.993	2181.292	-35.605
3300	829.552	1994.728	1339.582	2161.981	323.990	2239.370	-35.446
3400	831.025	2019.514	1359.217	2245.011	323.727	2297.388	-35.294
3500	832.382	2043.624	1378.429	2328.182	323.206	2355.402	-35.152
3600	833.635	2067.090	1397.234	2411.484	322.445	2413.500	-35.018
3700	834.794	2089.947	1415.648	2494.906	321.419	2471.640	-34.893
3800	835.867	2112.224	1433.687	2578.440	320.105	2529.760	-34.773
3900	836.864	2133.949	1451.365	2662.077	318.539	2587.882	-34.660
4000	837.790	2155.148	1468.696	2745.810	316.704	2646.154	-34.555
4100	838.653	2175.846	1485.692	2829.633	314.574	2704.417	-34.454
4200	839.458	2196.066	1502.366	2913.539	312.170	2762.728	-34.359
4300	840.210	2215.827	1518.729	2997.523	309.479	2821.030	-34.268
4400	840.914	2235.152	1534.793	3081.579	306.512	2879.471	-34.183
4500	841.573	2254.057	1550.567	3165.704	303.277	2938.028	-34.103
4600	842.191	2272.560	1566.062	3249.892	299.734	2996.661	-34.027
4700	842.772	2290.679	1581.287	3334.141	295.895	3055.288	-33.955
4800	843.318	2308.428	1596.252	3418.446	291.796	3114.081	-33.887
4900	843.832	2325.822	1610.964	3502.803	287.380	3172.858	-33.822
5000	844.317	2342.875	1625.432	3587.211	282.720	3231.876	-33.762

3.102. 1*H*-Indeno[1,2-*b*]anthracene



Other names: 2,3- β -Naphthofluorene
lin-Naphthofluorene

Formula: C₂₁H₁₄
Mass: 266.336 g/mol

CAS Number: 248-93-1

Point Group: C_s

Length: 16.08 Å
Width: 7.936 Å
Breadth: 4.176 Å
L/B Ratio: 2.026

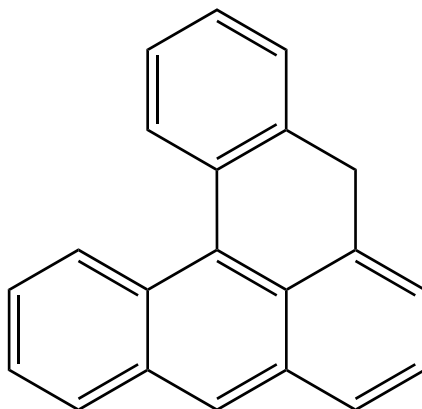
Cartesian coordinates:

C	-5.7936	0.2300	0.0000	C	1.3949	1.2449	0.0000	H	-4.8691	2.1629	-0.0000
C	-5.5977	-1.1807	0.0000	C	1.5925	-0.1890	-0.0000	H	-1.7485	-2.4508	0.0000
C	-4.3418	-1.7044	0.0000	C	2.7269	1.9413	0.0000	H	-2.4367	2.5012	-0.0000
C	-4.7279	1.0762	-0.0000	C	3.7082	0.8034	0.0000	H	0.6887	-2.1344	-0.0000
C	-3.3917	0.5614	-0.0000	C	3.0319	-0.4390	-0.0000	H	-0.0124	2.8620	0.0000
C	-3.1964	-0.8449	0.0000	C	3.7363	-1.6306	-0.0000	H	2.8511	2.5880	0.8883
C	-1.8975	-1.3639	0.0000	C	5.1321	-1.5742	-0.0000	H	2.8511	2.5880	-0.8883
C	-2.2832	1.4150	-0.0000	C	5.7971	-0.3541	0.0000	H	3.2106	-2.5909	-0.0000
C	-0.9877	0.8986	-0.0000	C	5.0892	0.8515	0.0000	H	5.7075	-2.5058	-0.0000
C	-0.7916	-0.5133	-0.0000	H	-6.8172	0.6185	0.0000	H	6.8919	-0.3332	0.0000
C	0.5424	-1.0484	-0.0000	H	-6.4768	-1.8334	0.0000	H	5.6175	1.8097	0.0000
C	0.1505	1.7789	0.0000	H	-4.1814	-2.7885	0.0000				

Table 3.102: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[1,2-*b*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.144	335.465	335.465	∞
100	91.719	326.542	679.033	-35.249	359.303	399.157	-208.494
200	175.948	414.469	524.889	-22.084	346.764	443.992	-115.956
250	225.755	459.030	507.241	-12.053	340.807	468.988	-97.988
298.15	274.830	502.993	502.993	0.000	335.465	494.173	-86.575
300	276.700	504.699	502.998	0.510	335.269	495.157	-86.213
350	325.993	551.089	506.550	15.589	330.313	522.207	-77.934
400	371.868	597.658	515.029	33.052	325.985	549.916	-71.810
450	413.522	643.906	526.784	52.705	322.223	578.137	-67.107
500	450.830	689.443	540.780	74.332	318.958	606.767	-63.387
600	513.592	777.410	572.952	122.675	313.660	664.854	-57.879
700	563.486	860.470	608.154	176.622	309.808	723.714	-54.003
800	603.731	938.433	644.618	235.052	307.226	783.025	-51.125
900	636.707	1011.508	681.368	297.126	305.748	842.588	-48.902
1000	664.077	1080.052	717.845	362.207	305.217	902.274	-47.129
1100	687.022	1144.453	753.730	429.794	305.458	961.981	-45.680
1200	706.408	1205.086	788.842	499.493	306.339	1021.623	-44.469
1300	722.895	1262.297	823.082	570.980	307.700	1081.180	-43.441
1400	736.999	1316.399	856.404	643.992	309.425	1140.622	-42.556
1500	749.128	1367.670	888.795	718.314	311.436	1199.930	-41.784
1600	759.612	1416.361	920.259	793.763	313.624	1259.091	-41.104
1700	768.718	1462.692	950.815	870.190	315.920	1318.092	-40.499
1800	776.663	1506.860	980.489	947.468	318.263	1377.007	-39.959
1900	783.627	1549.043	1009.311	1025.490	320.622	1435.750	-39.471
2000	789.758	1589.397	1037.314	1104.166	322.949	1494.389	-39.029
2100	795.177	1628.063	1064.531	1183.418	325.180	1552.903	-38.626
2200	799.986	1665.168	1090.995	1263.181	327.313	1611.317	-38.257
2300	804.269	1700.825	1116.739	1343.398	329.340	1669.633	-37.918
2400	808.099	1735.137	1141.795	1424.020	331.205	1727.828	-37.604
2500	811.534	1768.196	1166.194	1505.004	332.915	1786.037	-37.316
2600	814.625	1800.086	1189.965	1586.315	334.439	1844.090	-37.047
2700	817.416	1830.884	1213.136	1667.919	335.782	1902.142	-36.798
2800	819.944	1860.657	1235.733	1749.789	336.921	1960.169	-36.567
2900	822.238	1889.471	1257.781	1831.900	337.832	2018.115	-36.349
3000	824.328	1917.382	1279.305	1914.230	338.548	2076.053	-36.147
3100	826.235	1944.443	1300.327	1996.760	339.010	2133.913	-35.955
3200	827.981	1970.703	1320.868	2079.472	339.248	2191.818	-35.777
3300	829.582	1996.206	1340.948	2162.351	339.247	2249.749	-35.610
3400	831.053	2020.994	1360.587	2245.384	338.987	2307.619	-35.452
3500	832.409	2045.104	1379.802	2328.558	338.469	2365.484	-35.302
3600	833.660	2068.571	1398.610	2411.862	337.710	2423.434	-35.162
3700	834.818	2091.429	1417.027	2495.287	336.687	2481.427	-35.031
3800	835.890	2113.706	1435.069	2578.823	335.376	2539.398	-34.906
3900	836.885	2135.432	1452.749	2662.462	333.812	2597.372	-34.787
4000	837.811	2156.632	1470.082	2746.198	331.979	2655.496	-34.677
4100	838.673	2177.330	1487.081	2830.022	329.851	2713.610	-34.571
4200	839.477	2197.550	1503.757	2913.930	327.449	2771.773	-34.471
4300	840.228	2217.312	1520.122	2997.916	324.760	2829.927	-34.376
4400	840.931	2236.637	1536.188	3081.974	321.795	2888.219	-34.287
4500	841.589	2255.542	1551.964	3166.101	318.561	2946.627	-34.203
4600	842.207	2274.046	1567.461	3250.291	315.020	3005.112	-34.123
4700	842.787	2292.165	1582.689	3334.541	311.182	3063.590	-34.047
4800	843.333	2309.915	1597.655	3418.847	307.085	3122.234	-33.976
4900	843.846	2327.309	1612.369	3503.206	302.671	3180.862	-33.908
5000	844.331	2344.362	1626.839	3587.615	298.012	3239.733	-33.845

3.103. 5*H*-Dibenzo[*c,mn*]phenanthrene



Other names: Ceranthrene
H-Naphth[3,2,1-*de*]anthrene

Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 192-11-0
Point Group: C₁

Length: 11.96 Å
Width: 11.34 Å
Breadth: 5.462 Å
L/B Ratio: 1.054

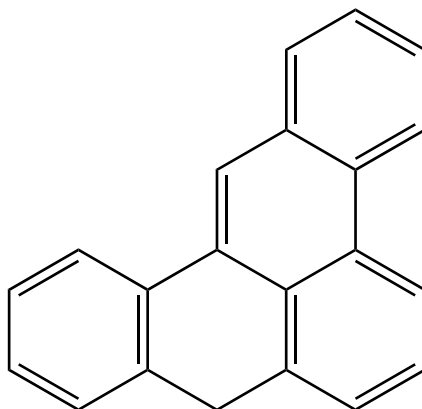
Cartesian coordinates:

C	1.3350	2.2163	0.5702	C	-2.3856	-1.3333	0.3190	H	-0.6087	2.8357	-0.5911
C	1.2406	0.9213	0.0446	C	-1.1499	-1.9733	0.2291	H	-3.2891	-1.9172	0.5342
C	2.4327	0.2660	-0.3082	C	-3.7687	0.6681	0.0759	H	-1.9530	-3.9606	0.6188
C	3.6595	0.9242	-0.2060	C	-3.8927	1.9964	-0.1829	H	0.2445	-5.1007	0.3546
C	3.7248	2.2233	0.2777	C	-2.7324	2.7783	-0.4381	H	2.2481	-3.8069	-0.3060
C	2.5580	2.8626	0.6813	C	-1.4944	2.2164	-0.3926	H	2.3969	-1.1628	-1.8838
C	2.4207	-1.1490	-0.7733	C	1.3094	-3.2703	-0.1274	H	3.3645	-1.6564	-0.4845
C	1.2460	-1.9125	-0.2677	C	0.1530	-4.0171	0.2278	H	4.5791	0.4055	-0.5008
C	0.0193	-1.2078	-0.0205	C	-1.0460	-3.3938	0.3805	H	4.6893	2.7354	0.3528
C	-0.0388	0.2029	-0.0439	H	-2.8544	3.8402	-0.6757	H	2.6022	3.8769	1.0913
C	-1.3059	0.8255	-0.1000	H	-4.8749	2.4791	-0.2069	H	0.4258	2.7394	0.8974
C	-2.4791	0.0419	0.0997	H	-4.6517	0.0460	0.2627				

Table 3.103: Table of thermodynamic data as a function of temperature for 5*H*-Dibenzo[*c,mn*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-40.459	363.821	363.821	∞
100	88.609	318.368	667.004	-34.864	388.044	428.715	-223.933
200	174.260	404.697	514.299	-21.920	375.283	474.465	-123.915
250	224.100	448.888	496.776	-11.972	369.243	499.960	-104.459
298.15	273.133	492.556	492.556	0.000	363.821	525.640	-92.088
300	275.002	494.251	492.561	0.507	363.621	526.643	-91.695
350	324.304	540.379	496.091	15.501	358.580	554.223	-82.711
400	370.250	586.727	504.525	32.881	354.170	582.473	-76.062
450	412.015	632.790	516.222	52.456	350.329	611.245	-70.950
500	449.448	678.175	530.155	74.010	346.992	640.435	-66.904
600	512.450	765.911	562.199	122.228	341.568	699.660	-60.910
700	562.535	848.811	597.282	176.070	337.611	759.680	-56.687
800	602.922	926.656	633.641	234.412	334.942	820.163	-53.550
900	636.004	999.642	670.296	296.412	333.388	880.908	-51.126
1000	663.457	1068.117	706.691	361.426	332.792	941.784	-49.193
1100	686.467	1132.461	742.502	428.955	332.974	1002.687	-47.613
1200	705.908	1193.049	777.548	498.601	333.802	1063.531	-46.293
1300	722.441	1250.222	811.729	570.040	335.116	1124.294	-45.174
1400	736.585	1304.291	844.999	643.009	336.797	1184.944	-44.210
1500	748.749	1355.536	877.342	717.291	338.769	1245.465	-43.370
1600	759.265	1404.203	908.762	792.704	340.920	1305.841	-42.630
1700	768.398	1450.513	939.279	869.098	343.184	1366.058	-41.973
1800	776.369	1494.664	968.917	946.345	345.496	1426.192	-41.386
1900	783.355	1536.832	997.706	1024.339	347.827	1486.155	-40.856
2000	789.506	1577.172	1025.678	1102.988	350.127	1546.017	-40.377
2100	794.943	1615.827	1052.866	1182.216	352.334	1605.753	-39.940
2200	799.768	1652.921	1079.304	1261.957	354.444	1665.391	-39.541
2300	804.067	1688.569	1105.024	1342.152	356.450	1724.932	-39.174
2400	807.909	1722.872	1130.058	1422.755	358.295	1784.354	-38.835
2500	811.357	1755.924	1154.435	1503.721	359.987	1843.790	-38.523
2600	814.460	1787.807	1178.186	1585.015	361.494	1903.070	-38.232
2700	817.261	1818.599	1201.338	1666.603	362.821	1962.350	-37.963
2800	819.797	1848.367	1223.918	1748.458	363.945	2021.606	-37.713
2900	822.101	1877.176	1245.950	1830.555	364.841	2080.781	-37.478
3000	824.198	1905.082	1267.458	1912.871	365.545	2139.949	-37.259
3100	826.113	1932.139	1288.465	1995.388	365.994	2199.039	-37.053
3200	827.865	1958.395	1308.992	2078.088	366.220	2258.175	-36.860
3300	829.472	1983.895	1329.060	2160.956	366.208	2317.337	-36.680
3400	830.949	2008.679	1348.686	2243.979	365.937	2376.438	-36.509
3500	832.310	2032.786	1367.889	2327.142	365.409	2435.535	-36.348
3600	833.567	2056.251	1386.685	2410.437	364.641	2494.717	-36.197
3700	834.728	2079.106	1405.092	2493.853	363.608	2553.941	-36.054
3800	835.805	2101.381	1423.123	2577.380	362.289	2613.145	-35.919
3900	836.805	2123.105	1440.794	2661.011	360.716	2672.352	-35.791
4000	837.734	2144.303	1458.118	2744.739	358.875	2731.708	-35.672
4100	838.599	2164.999	1475.108	2828.556	356.739	2791.056	-35.558
4200	839.407	2185.217	1491.775	2912.456	354.330	2850.452	-35.450
4300	840.161	2204.978	1508.132	2996.435	351.635	2909.839	-35.347
4400	840.866	2224.301	1524.190	3080.487	348.663	2969.364	-35.250
4500	841.528	2243.205	1539.959	3164.607	345.423	3029.006	-35.159
4600	842.148	2261.708	1555.449	3248.791	341.876	3088.725	-35.073
4700	842.730	2279.826	1570.669	3333.035	338.032	3148.437	-34.990
4800	843.278	2297.574	1585.629	3417.336	333.930	3208.315	-34.913
4900	843.794	2314.967	1600.336	3501.690	329.509	3268.178	-34.838
5000	844.280	2332.019	1614.800	3586.094	324.845	3328.282	-34.770

3.104. 8*H*-Dibenzo[*b,mn*]phenanthrene



Other names: 8*H*-meso- α -Naphthanthrene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 6542-08-1

Point Group: C_s

Length: 13.81 Å

Width: 10.33 Å

Breadth: 4.171 Å

L/B Ratio: 1.337

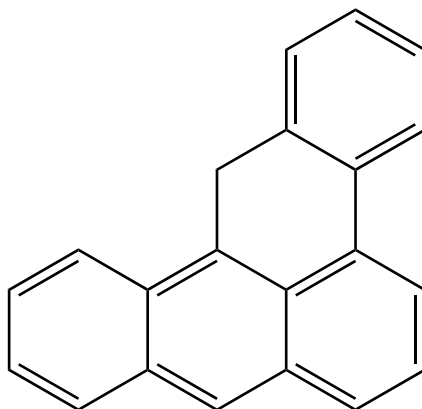
Cartesian coordinates:

C	-2.7477	-2.4065	0.0000	C	0.4627	-0.5217	0.0000	H	-4.8073	-3.0170	-0.0000
C	-3.7296	0.2043	0.0000	C	2.3652	1.7180	-0.0000	H	-0.0684	-2.5944	0.0000
C	-4.5987	-0.8623	0.0000	C	0.8899	1.9284	0.0000	H	1.1135	4.0690	0.0000
C	-4.1044	-2.1776	0.0000	C	2.8120	0.2972	0.0000	H	-1.3273	4.5123	0.0000
C	-2.3338	-0.0061	0.0000	C	1.9063	-0.7701	0.0000	H	-2.9437	2.6116	0.0000
C	-1.8424	-1.3222	0.0000	C	2.4017	-2.0814	0.0000	H	2.7992	2.2280	0.8859
C	-0.4298	-1.5532	0.0000	C	3.7658	-2.3267	0.0000	H	2.7992	2.2280	-0.8859
C	-1.3985	1.0972	0.0000	C	4.6629	-1.2618	0.0000	H	1.6883	-2.9197	0.0000
C	0.4112	3.2276	0.0000	C	4.1867	0.0410	0.0000	H	4.1371	-3.3566	0.0000
C	-0.9664	3.4787	0.0000	H	-2.3558	-3.4299	0.0000	H	5.7409	-1.4521	0.0000
C	-1.8580	2.4303	0.0000	H	-4.1036	1.2395	0.0000	H	4.8907	0.8810	-0.0000
C	-0.0133	0.8413	0.0000	H	-5.6804	-0.6931	0.0000				

Table 3.104: Table of thermodynamic data as a function of temperature for 8*H*-Dibenzo[*b,mn*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-40.975	321.826	321.826	∞
100	91.422	326.994	677.563	-35.057	345.856	385.665	-201.446
200	175.060	414.605	524.307	-21.940	333.268	430.469	-112.425
250	224.261	458.902	506.778	-11.969	327.252	455.465	-95.162
298.15	272.871	502.560	502.560	0.000	321.826	480.662	-84.208
300	274.726	504.254	502.565	0.507	321.625	481.647	-83.860
350	323.749	550.317	506.091	15.479	316.564	508.728	-75.922
400	369.531	596.578	514.511	32.827	312.121	536.483	-70.056
450	411.212	642.551	526.188	52.363	308.242	564.765	-65.555
500	448.616	687.850	540.097	73.877	304.863	593.469	-61.998
600	511.646	775.436	572.083	122.012	299.357	651.735	-56.737
700	561.808	858.216	607.106	175.777	295.324	710.808	-53.040
800	602.283	935.970	643.406	234.051	292.586	770.355	-50.298
900	635.448	1008.886	680.008	295.991	290.973	830.173	-48.181
1000	662.973	1077.306	716.352	360.953	290.324	890.127	-46.495
1100	686.045	1141.607	752.119	428.437	290.461	950.114	-45.116
1200	705.539	1202.160	787.124	498.043	291.250	1010.045	-43.965
1300	722.117	1259.306	821.269	569.448	292.529	1069.898	-42.988
1400	736.298	1313.353	854.505	642.387	294.180	1129.641	-42.147
1500	748.494	1364.578	886.817	716.642	296.124	1189.257	-41.413
1600	759.036	1413.230	918.210	792.031	298.251	1248.729	-40.766
1700	768.193	1459.527	948.702	868.403	300.494	1308.044	-40.190
1800	776.184	1503.667	978.317	945.631	302.786	1367.277	-39.677
1900	783.188	1545.825	1007.085	1023.607	305.099	1426.341	-39.212
2000	789.353	1586.157	1035.037	1102.240	307.384	1485.303	-38.791
2100	794.804	1624.805	1062.208	1181.453	309.576	1544.142	-38.408
2200	799.640	1661.893	1088.629	1261.180	311.673	1602.883	-38.056
2300	803.949	1697.535	1114.333	1341.364	313.667	1661.527	-37.734
2400	807.801	1731.834	1139.352	1421.955	315.501	1720.051	-37.435
2500	811.256	1764.881	1163.717	1502.911	317.182	1778.592	-37.161
2600	814.366	1796.761	1187.455	1584.195	318.680	1836.976	-36.905
2700	817.174	1827.549	1210.595	1665.774	319.997	1895.362	-36.667
2800	819.717	1857.314	1233.164	1747.621	321.113	1953.722	-36.446
2900	822.025	1886.120	1255.186	1829.710	322.001	2012.003	-36.239
3000	824.127	1914.024	1276.684	1912.019	322.698	2070.276	-36.046
3100	826.046	1941.079	1297.682	1994.529	323.140	2128.473	-35.864
3200	827.802	1967.333	1318.200	2077.223	323.360	2186.714	-35.694
3300	829.413	1992.830	1338.259	2160.085	323.341	2244.983	-35.534
3400	830.894	2017.613	1357.878	2243.101	323.065	2303.190	-35.383
3500	832.258	2041.719	1377.073	2326.260	322.531	2361.394	-35.241
3600	833.517	2065.182	1395.863	2409.549	321.758	2419.683	-35.108
3700	834.681	2088.036	1414.263	2492.960	320.721	2478.014	-34.983
3800	835.760	2110.310	1432.288	2576.482	319.396	2536.326	-34.864
3900	836.762	2132.032	1449.953	2660.109	317.819	2594.639	-34.751
4000	837.693	2153.229	1467.271	2743.833	315.974	2653.103	-34.645
4100	838.561	2173.924	1484.255	2827.646	313.835	2711.558	-34.545
4200	839.370	2194.142	1500.917	2911.543	311.422	2770.061	-34.450
4300	840.126	2213.901	1517.269	2995.518	308.723	2828.556	-34.359
4400	840.833	2233.224	1533.322	3079.566	305.747	2887.189	-34.275
4500	841.495	2252.127	1549.086	3163.683	302.504	2945.939	-34.195
4600	842.117	2270.629	1564.572	3247.864	298.954	3004.766	-34.119
4700	842.701	2288.746	1579.788	3332.105	295.107	3063.585	-34.047
4800	843.250	2306.494	1594.743	3416.403	291.002	3122.572	-33.980
4900	843.766	2323.886	1609.447	3500.754	286.579	3181.542	-33.915
5000	844.254	2340.937	1623.906	3585.155	281.912	3240.755	-33.855

3.105. 1*H*-Dibenzo[*b,mn*]phenanthrene



Other names: 1*H*-meso- α -Naphthanthrene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 198-30-1

Point Group: C_s

Length: 13.86 Å

Width: 10.30 Å

Breadth: 4.176 Å

L/B Ratio: 1.346

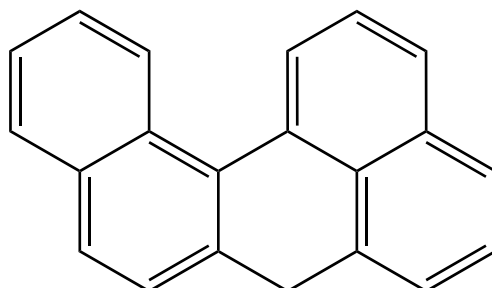
Cartesian coordinates:

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C	4.7160	-1.0931	-0.0000	C	-1.4001	1.0833	0.0000	H	2.9798	2.5483	0.0000
C	4.2140	0.1704	-0.0000	C	-0.4054	-1.6668	0.0000	H	1.1075	4.0869	0.0000
C	2.4864	-2.0308	0.0000	C	-1.8610	-1.3531	0.0000	H	-1.3487	4.4891	0.0000
C	1.9120	-0.7166	0.0000	C	-2.3387	-0.0385	0.0000	H	-2.9309	2.5807	0.0000
C	2.7985	0.3941	0.0000	C	-3.7225	0.1844	-0.0000	H	-0.1868	-2.2977	0.8885
C	2.2906	1.6946	0.0000	C	-4.6122	-0.8781	-0.0000	H	-0.1868	-2.2977	-0.8885
C	0.9138	1.9160	0.0000	C	-4.1325	-2.1858	-0.0000	H	-4.0939	1.2208	-0.0000
C	0.3974	3.2522	0.0000	C	-2.7654	-2.4199	0.0000	H	-5.6906	-0.6898	-0.0000
C	-0.9442	3.4717	0.0000	H	4.2642	-3.2180	-0.0000	H	-4.8332	-3.0269	-0.0000
C	-1.8488	2.3778	0.0000	H	5.7963	-1.2707	-0.0000	H	-2.3860	-3.4481	0.0000
C	0.5193	-0.4959	0.0000	H	4.8788	1.0418	-0.0000				

Table 3.105: Table of thermodynamic data as a function of temperature for 1*H*-Dibenzo[*b,mn*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.189	346.013	346.013	∞
100	91.833	331.240	683.109	-35.187	369.913	409.297	-213.791
200	175.768	419.215	529.296	-22.016	357.380	453.658	-118.481
250	225.049	463.680	511.708	-12.007	351.401	478.420	-99.958
298.15	273.647	507.477	507.477	0.000	346.013	503.384	-88.189
300	275.501	509.175	507.482	0.508	345.814	504.359	-87.815
350	324.457	555.353	511.017	15.518	340.790	531.191	-79.274
400	370.155	601.704	519.457	32.899	336.380	558.693	-72.956
450	411.753	647.746	531.158	52.464	332.531	586.716	-68.103
500	449.083	693.097	545.091	74.003	329.177	615.159	-64.264
600	512.003	780.758	577.127	122.179	323.712	672.896	-58.580
700	562.094	863.588	612.193	175.976	319.710	731.434	-54.579
800	602.522	941.377	648.531	234.276	316.999	790.443	-51.610
900	635.655	1014.319	685.166	296.238	315.407	849.718	-49.315
1000	663.157	1082.759	721.539	361.220	314.778	909.128	-47.487
1100	686.211	1147.077	757.330	428.722	314.933	968.569	-45.993
1200	705.689	1207.644	792.358	498.343	315.738	1027.952	-44.745
1300	722.254	1264.801	826.522	569.763	317.031	1087.256	-43.686
1400	736.424	1318.858	859.776	642.715	318.695	1146.450	-42.774
1500	748.610	1370.092	892.104	716.981	320.652	1205.514	-41.979
1600	759.143	1418.750	923.512	792.382	322.790	1264.434	-41.279
1700	768.292	1465.054	954.016	868.764	325.042	1323.197	-40.656
1800	776.275	1509.199	983.643	946.001	327.344	1381.878	-40.100
1900	783.272	1551.362	1012.422	1023.986	329.666	1440.388	-39.598
2000	789.432	1591.698	1040.384	1102.628	331.959	1498.796	-39.144
2100	794.876	1630.349	1067.564	1181.848	334.159	1557.081	-38.729
2200	799.708	1667.441	1093.994	1261.582	336.263	1615.267	-38.351
2300	804.012	1703.086	1119.706	1341.772	338.263	1673.356	-38.002
2400	807.860	1737.387	1144.733	1422.370	340.103	1731.325	-37.681
2500	811.311	1770.437	1169.104	1503.331	341.790	1789.310	-37.385
2600	814.418	1802.318	1192.849	1584.620	343.293	1847.139	-37.109
2700	817.223	1833.108	1215.995	1666.205	344.615	1904.968	-36.853
2800	819.762	1862.875	1238.570	1748.056	345.735	1962.773	-36.615
2900	822.068	1891.683	1260.597	1830.149	346.629	2020.498	-36.392
3000	824.168	1919.588	1282.101	1912.463	347.329	2078.215	-36.184
3100	826.085	1946.644	1303.103	1994.977	347.775	2135.854	-35.988
3200	827.839	1972.899	1323.626	2077.674	347.999	2193.540	-35.805
3300	829.447	1998.398	1343.689	2160.540	347.984	2251.251	-35.634
3400	830.926	2023.182	1363.312	2243.559	347.711	2308.902	-35.471
3500	832.289	2047.289	1382.511	2326.721	347.180	2366.549	-35.318
3600	833.546	2070.753	1401.304	2410.014	346.410	2424.281	-35.175
3700	834.709	2093.607	1419.708	2493.427	345.375	2482.055	-35.040
3800	835.787	2115.882	1437.736	2576.953	344.054	2539.809	-34.911
3900	836.787	2137.605	1455.404	2660.582	342.479	2597.565	-34.790
4000	837.718	2158.802	1472.725	2744.308	340.637	2655.472	-34.676
4100	838.584	2179.499	1489.712	2828.123	338.500	2713.369	-34.568
4200	839.392	2199.716	1506.377	2912.023	336.089	2771.315	-34.466
4300	840.147	2219.476	1522.732	2996.000	333.392	2829.252	-34.368
4400	840.853	2238.799	1538.788	3080.050	330.419	2887.328	-34.276
4500	841.515	2257.703	1554.554	3164.169	327.177	2945.520	-34.190
4600	842.135	2276.205	1570.042	3248.352	323.629	3003.789	-34.108
4700	842.718	2294.323	1585.260	3332.595	319.784	3062.051	-34.030
4800	843.267	2312.071	1600.218	3416.895	315.681	3120.480	-33.957
4900	843.783	2329.464	1614.923	3501.247	311.260	3178.893	-33.887
5000	844.270	2346.515	1629.385	3585.650	306.594	3237.547	-33.822

3.106. 7H-Dibenz[*a,k*]anthracene



Other names: Benzobenzanthrene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 194-83-2

Point Group: C₁

Length: 12.99 Å

Width: 9.380 Å

Breadth: 5.128 Å

L/B Ratio: 1.385

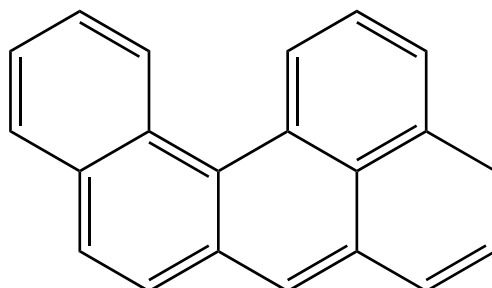
Cartesian coordinates:

C	-4.6430	-1.0209	-0.4343	C	3.2990	1.8043	-0.4207	H	-3.8030	-2.9688	-0.8760
C	-4.3703	0.2839	-0.1278	C	4.3836	0.9265	-0.6318	H	-3.6137	2.7926	0.3660
C	-2.2842	-1.5355	-0.4020	C	4.2301	-0.4199	-0.4367	H	-1.2703	3.6105	0.4663
C	-3.5799	-1.9348	-0.5927	C	0.5496	-0.6277	0.2906	H	0.9742	3.1263	-0.3736
C	-1.9591	-0.1993	-0.0390	C	1.8518	-0.0889	0.0327	H	1.1623	2.6326	1.3174
C	-3.0295	0.7200	0.0476	C	2.9640	-0.9500	-0.0725	H	3.4575	2.8839	-0.5194
C	-2.7708	2.0979	0.2762	C	2.8086	-2.3301	0.2244	H	5.3529	1.3397	-0.9291
C	-1.4843	2.5422	0.3444	C	1.5903	-2.8026	0.6267	H	5.0770	-1.1051	-0.5542
C	-0.6140	0.2655	0.1808	C	0.4623	-1.9539	0.6547	H	3.6777	-2.9930	0.1494
C	-0.3991	1.6304	0.2726	H	-5.6738	-1.3626	-0.5710	H	1.4671	-3.8526	0.9123
C	0.9614	2.2414	0.2972	H	-5.1806	1.0146	-0.0229	H	-0.5019	-2.3898	0.9502
C	2.0629	1.3129	-0.0713	H	-1.4763	-2.2665	-0.5430				

Table 3.106: Table of thermodynamic data as a function of temperature for 7H-Dibenz[*a,k*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-40.677	354.313	354.313	∞
100	89.537	322.771	672.033	-34.926	378.474	418.705	-218.704
200	174.497	409.428	519.126	-21.939	365.757	463.992	-121.180
250	224.295	453.668	501.590	-11.980	359.728	489.249	-102.221
298.15	273.277	497.366	497.366	0.000	354.313	514.698	-90.171
300	275.144	499.063	497.372	0.507	354.113	515.692	-89.788
350	324.392	545.209	500.904	15.507	349.079	543.031	-81.041
400	370.293	591.565	509.340	32.890	344.671	571.039	-74.569
450	412.025	637.631	521.040	52.466	340.832	599.570	-69.595
500	449.436	683.016	534.975	74.020	337.495	628.517	-65.659
600	512.416	770.748	567.022	122.236	332.069	687.259	-59.830
700	562.496	853.641	602.107	176.074	328.108	746.795	-55.725
800	602.885	931.482	638.466	234.413	325.435	806.795	-52.677
900	635.972	1004.464	675.121	296.408	323.878	867.058	-50.322
1000	663.429	1072.935	711.515	361.420	323.278	927.452	-48.444
1100	686.444	1137.277	747.326	428.947	323.458	987.874	-46.909
1200	705.889	1197.863	782.371	498.590	324.284	1048.236	-45.628
1300	722.426	1255.035	816.552	570.028	325.596	1108.517	-44.540
1400	736.572	1309.103	849.821	642.996	327.276	1168.687	-43.603
1500	748.739	1360.347	882.163	717.276	329.246	1228.726	-42.787
1600	759.255	1409.013	913.583	792.688	331.396	1288.621	-42.068
1700	768.390	1455.323	944.099	869.081	333.659	1348.357	-41.429
1800	776.362	1499.474	973.736	946.328	335.971	1408.010	-40.859
1900	783.349	1541.641	1002.524	1024.321	338.301	1467.492	-40.343
2000	789.501	1581.981	1030.496	1102.970	340.601	1526.873	-39.877
2100	794.939	1620.635	1057.684	1182.197	342.807	1586.129	-39.452
2200	799.764	1657.729	1084.121	1261.937	344.917	1645.286	-39.063
2300	804.063	1693.377	1109.841	1342.133	346.923	1704.346	-38.706
2400	807.906	1727.680	1134.874	1422.735	348.768	1763.286	-38.376
2500	811.354	1760.732	1159.251	1503.701	350.459	1822.242	-38.073
2600	814.457	1792.615	1183.002	1584.994	351.966	1881.041	-37.790
2700	817.259	1823.406	1206.154	1666.582	353.292	1939.841	-37.528
2800	819.795	1853.175	1228.733	1748.437	354.416	1998.616	-37.284
2900	822.099	1881.983	1250.765	1830.533	355.312	2057.310	-37.055
3000	824.197	1909.890	1272.273	1912.850	356.016	2115.997	-36.842
3100	826.111	1936.946	1293.280	1995.366	356.465	2174.607	-36.641
3200	827.863	1963.203	1313.807	2078.067	356.691	2233.262	-36.454
3300	829.471	1988.702	1333.874	2160.934	356.678	2291.943	-36.278
3400	830.948	2013.487	1353.499	2243.956	356.407	2350.563	-36.111
3500	832.309	2037.594	1372.702	2327.120	355.879	2409.180	-35.954
3600	833.565	2061.058	1391.499	2410.415	355.111	2467.881	-35.807
3700	834.727	2083.913	1409.905	2493.830	354.078	2526.625	-35.669
3800	835.804	2106.188	1427.937	2577.357	352.758	2585.348	-35.537
3900	836.804	2127.912	1445.607	2660.988	351.185	2644.073	-35.413
4000	837.733	2149.110	1462.931	2744.716	349.345	2702.949	-35.296
4100	838.599	2169.806	1479.920	2828.533	347.209	2761.816	-35.185
4200	839.406	2190.024	1496.588	2912.433	344.799	2820.731	-35.080
4300	840.160	2209.785	1512.945	2996.412	342.104	2879.637	-34.980
4400	840.866	2229.108	1529.003	3080.464	339.132	2938.683	-34.886
4500	841.527	2248.012	1544.771	3164.584	335.892	2997.844	-34.797
4600	842.147	2266.515	1560.261	3248.768	332.345	3057.082	-34.714
4700	842.729	2284.633	1575.481	3333.012	328.501	3116.313	-34.633
4800	843.277	2302.381	1590.441	3417.313	324.399	3175.711	-34.558
4900	843.793	2319.774	1605.148	3501.666	319.978	3235.092	-34.486
5000	844.279	2336.826	1619.612	3586.070	315.314	3294.716	-34.419

3.107. 4*H*-Dibenz[*a,k*]anthracene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 194-85-4
Point Group: C₁

Length: 13.05 Å
Width: 9.446 Å
Breadth: 4.824 Å
L/B Ratio: 1.382

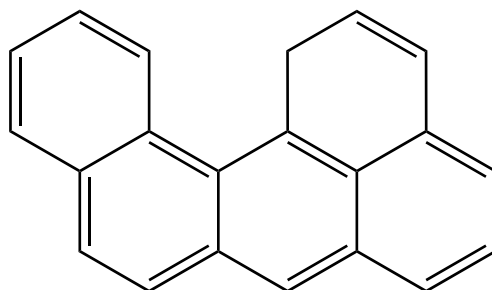
Cartesian coordinates:

C	2.9603	-0.9585	-0.0133	C	-3.0357	0.7413	-0.1423	H	-3.9469	-2.8832	0.8908
C	2.8022	-2.3089	-0.2490	C	-1.9943	-0.1895	0.0644	H	-3.5620	2.8170	-0.5565
C	1.5245	-2.8297	-0.4980	C	-4.3891	0.3337	-0.0706	H	-1.2129	3.6174	-0.4117
C	0.4197	-2.0144	-0.4533	C	-4.7117	-0.9561	0.2689	H	1.0745	3.2379	0.0105
C	0.5269	-0.6362	-0.1496	C	-3.6862	-1.8689	0.5709	H	3.6728	-2.9738	-0.2617
C	1.8275	-0.1039	0.0018	C	-2.3685	-1.4933	0.4743	H	1.4150	-3.8934	-0.7342
C	2.0128	1.3147	0.1187	C	4.3377	-0.4259	0.2100	H	-0.5652	-2.4472	-0.6745
C	0.9400	2.1489	-0.0055	C	4.4216	1.0444	0.3756	H	3.4478	2.9299	0.4457
C	-0.3803	1.6240	-0.1266	C	3.3517	1.8442	0.3263	H	5.4238	1.4548	0.5432
C	-0.6193	0.2458	-0.0694	H	-5.7571	-1.2758	0.3246	H	4.7711	-0.9128	1.1087
C	-1.4537	2.5530	-0.3059	H	-5.1763	1.0673	-0.2797	H	4.9872	-0.7249	-0.6394
C	-2.7366	2.1206	-0.3696	H	-1.5903	-2.2226	0.7371				

Table 3.107: Table of thermodynamic data as a function of temperature for 4*H*-Dibenz[*a,k*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-40.880	368.443	368.443	∞
100	90.261	322.645	673.633	-35.099	392.431	432.675	-226.001
200	175.438	409.881	520.017	-22.027	379.799	477.944	-124.824
250	225.201	454.328	502.414	-12.022	373.816	503.173	-105.130
298.15	274.070	498.178	498.178	0.000	368.443	528.586	-92.604
300	275.931	499.879	498.183	0.509	368.245	529.579	-92.206
350	325.022	546.134	501.724	15.544	363.246	556.873	-83.107
400	370.765	592.565	510.178	32.955	358.865	584.834	-76.370
450	412.356	638.678	521.899	52.551	355.046	613.313	-71.190
500	449.654	684.091	535.854	74.119	351.722	642.207	-67.090
600	512.486	771.849	567.937	122.347	346.310	700.840	-61.012
700	562.494	854.747	603.049	176.189	342.352	760.265	-56.731
800	602.856	932.585	639.428	234.525	339.677	820.155	-53.550
900	635.938	1005.563	676.099	296.518	338.117	880.308	-51.091
1000	663.399	1074.031	712.504	361.526	337.514	940.592	-49.130
1100	686.421	1138.370	748.325	429.050	337.691	1000.905	-47.528
1200	705.874	1198.954	783.378	498.692	338.515	1061.158	-46.190
1300	722.418	1256.125	817.565	570.128	339.826	1121.330	-45.055
1400	736.570	1310.193	850.839	643.096	341.505	1181.390	-44.077
1500	748.740	1361.437	883.186	717.376	343.476	1241.321	-43.226
1600	759.261	1410.103	914.610	792.789	345.626	1301.106	-42.476
1700	768.398	1456.414	945.130	869.182	347.890	1360.734	-41.809
1800	776.371	1500.565	974.771	946.429	350.202	1420.277	-41.215
1900	783.360	1542.732	1003.562	1024.424	352.533	1479.651	-40.678
2000	789.512	1583.073	1031.536	1103.074	354.834	1538.922	-40.192
2100	794.951	1621.728	1058.727	1182.302	357.042	1598.069	-39.749
2200	799.776	1658.823	1085.167	1262.043	359.153	1657.117	-39.344
2300	804.075	1694.471	1110.888	1342.240	361.160	1716.067	-38.972
2400	807.918	1728.775	1135.923	1422.843	363.006	1774.898	-38.629
2500	811.366	1761.827	1160.302	1503.811	364.698	1833.744	-38.313
2600	814.469	1793.710	1184.055	1585.105	366.207	1892.434	-38.019
2700	817.270	1824.502	1207.208	1666.694	367.534	1951.124	-37.746
2800	819.807	1854.271	1229.789	1748.550	368.659	2009.790	-37.492
2900	822.110	1883.080	1251.822	1830.648	369.557	2068.374	-37.255
3000	824.207	1910.987	1273.331	1912.965	370.261	2126.951	-37.033
3100	826.121	1938.044	1294.340	1995.483	370.711	2185.451	-36.824
3200	827.873	1964.300	1314.868	2078.184	370.938	2243.997	-36.629
3300	829.480	1989.800	1334.936	2161.053	370.927	2302.568	-36.446
3400	830.957	2014.585	1354.563	2244.076	370.657	2361.078	-36.273
3500	832.318	2038.692	1373.766	2327.241	370.129	2419.585	-36.110
3600	833.574	2062.157	1392.564	2410.536	369.362	2478.176	-35.957
3700	834.736	2085.012	1410.971	2493.952	368.330	2536.810	-35.813
3800	835.812	2107.288	1429.003	2577.480	367.011	2595.424	-35.676
3900	836.811	2129.011	1446.675	2661.112	365.439	2654.039	-35.546
4000	837.740	2150.209	1463.999	2744.840	363.599	2712.805	-35.425
4100	838.606	2170.906	1480.990	2828.658	361.464	2771.562	-35.309
4200	839.413	2191.124	1497.658	2912.559	359.055	2830.367	-35.200
4300	840.167	2210.885	1514.016	2996.539	356.361	2889.163	-35.096
4400	840.872	2230.208	1530.074	3080.591	353.389	2948.098	-34.998
4500	841.533	2249.113	1545.843	3164.712	350.150	3007.150	-34.905
4600	842.153	2267.615	1561.334	3248.896	346.603	3066.278	-34.818
4700	842.735	2285.733	1576.554	3333.141	342.760	3125.399	-34.734
4800	843.283	2303.481	1591.514	3417.442	338.658	3184.686	-34.656
4900	843.798	2320.875	1606.222	3501.796	334.238	3243.958	-34.580
5000	844.284	2337.927	1620.686	3586.201	329.575	3303.471	-34.510

3.108. 1*H*-Dibenz[*a,k*]anthracene



Other names: Dehydro-8,9-trimethylene-1,2-benzanthracene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 194-84-3

Point Group: C_s

Length: 13.23 Å

Width: 9.563 Å

Breadth: 4.181 Å

L/B Ratio: 1.383

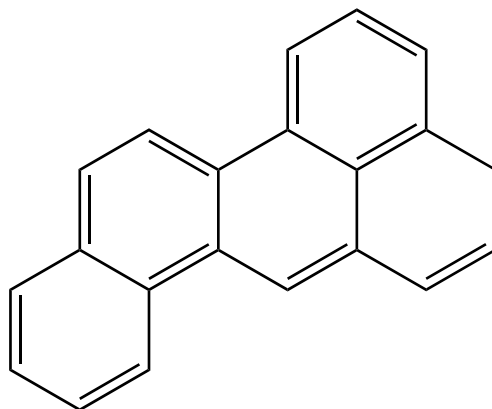
Cartesian coordinates:

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C	4.3707	0.4734	0.0000	C	-4.4755	0.9798	0.0000	H	3.4962	2.9508	0.0000
C	2.4435	-1.5047	0.0000	C	-4.2806	-0.4209	0.0000	H	1.1250	3.6744	0.0000
C	3.7829	-1.8413	0.0000	C	-0.5318	-0.6263	0.0000	H	-1.1349	3.2332	0.0000
C	1.9955	-0.1682	0.0000	C	-1.8548	-0.1068	0.0000	H	-3.5308	2.9055	0.0000
C	3.0066	0.8195	0.0000	C	-3.0145	-0.9545	0.0000	H	-5.4963	1.3756	0.0000
C	2.6780	2.2212	0.0000	C	-2.8410	-2.3959	0.0000	H	-5.1578	-1.0782	0.0000
C	1.3922	2.6107	0.0000	C	-1.6177	-2.9293	0.0000	H	-3.7421	-3.0199	0.0000
C	0.5814	0.2342	0.0000	C	-0.3835	-2.1135	0.0000	H	-1.4729	-4.0158	-0.0000
C	0.3208	1.6423	0.0000	H	5.8239	-1.1175	0.0000	H	0.2152	-2.4140	0.8910
C	-0.9683	2.1479	0.0000	H	5.1246	1.2697	0.0000	H	0.2152	-2.4140	-0.8910
C	-2.0747	1.2889	0.0000	H	1.7285	-2.3383	0.0000				

Table 3.108: Table of thermodynamic data as a function of temperature for 1*H*-Dibenz[*a,k*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-40.619	389.459	389.459	∞
100	88.195	324.581	673.534	-34.895	413.651	453.701	-236.984
200	174.533	410.792	520.616	-21.965	400.877	498.840	-130.281
250	224.589	455.072	503.058	-11.996	394.858	524.028	-109.487
298.15	273.627	498.829	498.829	0.000	389.459	549.408	-96.252
300	275.493	500.527	498.834	0.508	389.260	550.399	-95.831
350	324.682	546.724	502.370	15.524	384.242	577.663	-86.210
400	370.476	593.112	510.814	32.919	379.846	605.595	-79.081
450	412.094	639.193	522.523	52.501	376.013	634.048	-73.597
500	449.405	684.580	536.467	74.056	372.676	662.917	-69.253
600	512.245	772.292	568.525	122.261	367.240	721.503	-62.811
700	562.253	855.153	603.613	176.078	363.258	780.886	-58.269
800	602.614	932.959	639.971	234.391	360.559	840.737	-54.893
900	635.697	1005.909	676.621	296.359	358.974	900.854	-52.283
1000	663.163	1074.351	713.008	361.343	358.347	961.105	-50.202
1100	686.192	1138.669	748.811	428.844	358.501	1021.386	-48.501
1200	705.654	1199.233	783.847	498.463	359.303	1081.611	-47.080
1300	722.208	1256.387	818.019	569.878	360.592	1141.756	-45.875
1400	736.371	1310.440	851.279	642.825	362.251	1201.791	-44.838
1500	748.553	1361.670	883.612	717.086	364.202	1261.697	-43.935
1600	759.084	1410.325	915.024	792.481	366.335	1321.460	-43.140
1700	768.232	1456.625	945.532	868.857	368.581	1381.066	-42.434
1800	776.216	1500.767	975.162	946.088	370.877	1440.589	-41.804
1900	783.215	1542.926	1003.943	1024.067	373.193	1499.942	-41.235
2000	789.376	1583.260	1031.908	1102.703	375.480	1559.195	-40.721
2100	794.823	1621.908	1059.090	1181.919	377.675	1618.323	-40.253
2200	799.657	1658.997	1085.521	1261.647	379.773	1677.353	-39.825
2300	803.963	1694.640	1111.234	1341.832	381.768	1736.287	-39.432
2400	807.813	1728.939	1136.262	1422.425	383.604	1795.101	-39.069
2500	811.267	1761.987	1160.634	1503.382	385.286	1853.931	-38.735
2600	814.375	1793.867	1184.380	1584.667	386.785	1912.605	-38.424
2700	817.182	1824.655	1207.527	1666.247	388.103	1971.279	-38.136
2800	819.723	1854.421	1230.102	1748.094	389.219	2029.930	-37.868
2900	822.031	1883.227	1252.129	1830.184	390.109	2088.499	-37.617
3000	824.133	1911.131	1273.633	1912.494	390.806	2147.062	-37.383
3100	826.051	1938.186	1294.636	1995.004	391.248	2205.548	-37.162
3200	827.807	1964.440	1315.159	2077.698	391.468	2264.079	-36.957
3300	829.417	1989.938	1335.223	2160.561	391.451	2322.636	-36.764
3400	830.897	2014.721	1354.845	2243.577	391.174	2381.133	-36.581
3500	832.261	2038.827	1374.045	2326.736	390.641	2439.626	-36.409
3600	833.519	2062.290	1392.838	2410.026	389.868	2498.204	-36.247
3700	834.684	2085.144	1411.242	2493.437	388.831	2556.825	-36.095
3800	835.763	2107.418	1429.270	2576.960	387.507	2615.425	-35.951
3900	836.764	2129.140	1446.938	2660.587	385.930	2674.028	-35.814
4000	837.695	2150.337	1464.259	2744.310	384.085	2732.781	-35.686
4100	838.562	2171.033	1481.246	2828.124	381.946	2791.525	-35.564
4200	839.371	2191.250	1497.912	2912.021	379.533	2850.318	-35.448
4300	840.127	2211.010	1514.266	2995.996	376.834	2909.101	-35.338
4400	840.834	2230.332	1530.322	3080.045	373.859	2968.024	-35.234
4500	841.497	2249.235	1546.088	3164.162	370.616	3027.063	-35.137
4600	842.118	2267.737	1561.576	3248.343	367.066	3086.179	-35.044
4700	842.702	2285.855	1576.794	3332.584	363.219	3145.287	-34.955
4800	843.250	2303.602	1591.752	3416.882	359.114	3204.563	-34.872
4900	843.767	2320.995	1606.457	3501.233	354.691	3263.823	-34.792
5000	844.254	2338.046	1620.919	3585.634	350.024	3323.324	-34.718

3.109. 4*H*-Benzo[*hi*]chrysene



Formula: C₂₁H₁₄
Mass: 266.336 g/mol
CAS Number: 216-54-6
Point Group: C_s

Length: 13.76 Å
Width: 9.211 Å
Breadth: 4.169 Å
L/B Ratio: 1.493

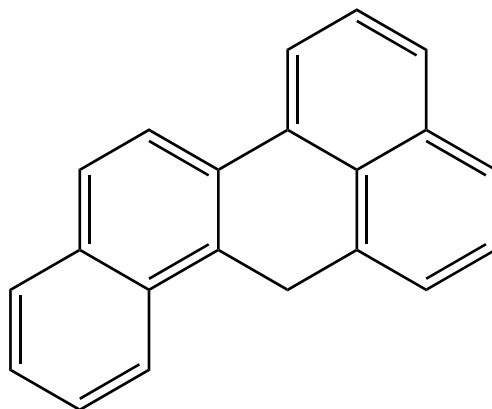
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C	4.3235	1.7139	0.0000	C	-4.2286	1.2046	0.0000	H	3.0583	-2.9666	0.0000
C	2.9528	1.6380	-0.0000	C	-1.1771	-1.0914	-0.0000	H	0.5515	2.4278	-0.0000
C	3.0777	-0.7887	0.0000	C	-1.9606	0.0781	-0.0000	H	-1.6296	3.5246	-0.0000
C	2.2983	0.3828	-0.0000	C	-3.3759	-0.0207	0.0000	H	-4.0912	3.3964	0.0000
C	1.0792	-2.1556	-0.0000	C	-3.9763	-1.2633	0.0000	H	-4.8977	1.1823	-0.8856
C	2.4344	-2.0656	0.0000	C	-3.1950	-2.4313	0.0000	H	-4.8977	1.1823	0.8856
C	0.2596	-0.9838	-0.0000	C	-1.8243	-2.3496	-0.0000	H	-5.0689	-1.3458	0.0000
C	0.8606	0.2768	-0.0000	H	5.0864	-1.6102	0.0000	H	-3.6910	-3.4074	0.0000
C	0.0468	1.4482	-0.0000	H	6.1918	0.6170	0.0000	H	-1.2043	-3.2588	-0.0000
C	-1.3173	1.3614	-0.0000	H	4.8236	2.6879	0.0000				

Table 3.109: Table of thermodynamic data as a function of temperature for 4*H*-Benzo[*hi*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-41.086	343.749	343.749	∞
100	91.634	326.925	678.472	-35.155	367.681	407.496	-212.850
200	175.623	414.728	524.770	-22.008	355.123	452.299	-118.126
250	224.985	459.171	507.187	-12.004	349.140	477.285	-99.721
298.15	273.571	502.957	502.957	0.000	343.749	502.467	-88.028
300	275.423	504.655	502.962	0.508	343.549	503.451	-87.657
350	324.310	550.816	506.496	15.512	338.519	530.509	-79.172
400	369.922	597.142	514.932	32.884	334.100	558.238	-72.897
450	411.444	643.151	526.628	52.436	330.237	586.490	-68.077
500	448.715	688.467	540.553	73.957	326.867	615.164	-64.264
600	511.571	776.054	572.567	122.092	321.361	673.368	-58.621
700	561.652	858.816	607.608	175.846	317.315	732.380	-54.650
800	602.099	936.547	643.919	234.103	314.560	791.868	-51.703
900	635.263	1009.441	680.526	296.024	312.928	851.629	-49.426
1000	662.798	1077.842	716.874	360.968	312.262	911.529	-47.612
1100	685.887	1142.127	752.641	428.435	312.382	971.463	-46.130
1200	705.396	1202.667	787.645	498.026	313.156	1031.342	-44.892
1300	721.990	1259.802	821.788	569.418	314.421	1091.145	-43.842
1400	736.185	1313.840	855.022	642.344	316.060	1150.840	-42.937
1500	748.393	1365.058	887.332	716.588	317.994	1210.407	-42.149
1600	758.946	1413.703	918.723	791.968	320.111	1269.831	-41.455
1700	768.112	1459.995	949.212	868.331	322.345	1329.099	-40.837
1800	776.111	1504.131	978.825	945.551	324.630	1388.286	-40.286
1900	783.122	1546.285	1007.590	1023.521	326.936	1447.303	-39.788
2000	789.293	1586.614	1035.540	1102.148	329.214	1506.220	-39.338
2100	794.749	1625.259	1062.708	1181.355	331.401	1565.013	-38.927
2200	799.590	1662.344	1089.127	1261.077	333.493	1623.708	-38.551
2300	803.903	1697.985	1114.830	1341.256	335.481	1682.307	-38.206
2400	807.759	1732.281	1139.847	1421.843	337.311	1740.787	-37.886
2500	811.217	1765.327	1164.209	1502.794	338.988	1799.283	-37.593
2600	814.330	1797.205	1187.946	1584.074	340.482	1857.623	-37.319
2700	817.141	1827.992	1211.084	1665.650	341.796	1915.964	-37.066
2800	819.685	1857.756	1233.651	1747.494	342.908	1974.280	-36.830
2900	821.996	1886.561	1255.671	1829.580	343.794	2032.517	-36.609
3000	824.100	1914.464	1277.169	1911.886	344.488	2090.746	-36.402
3100	826.021	1941.518	1298.165	1994.394	344.927	2148.898	-36.208
3200	827.779	1967.771	1318.682	2077.085	345.144	2207.096	-36.026
3300	829.391	1993.268	1338.740	2159.945	345.124	2265.321	-35.856
3400	830.873	2018.050	1358.357	2242.959	344.845	2323.485	-35.695
3500	832.238	2042.155	1377.551	2326.115	344.310	2381.645	-35.543
3600	833.498	2065.618	1396.339	2409.403	343.534	2439.890	-35.401
3700	834.664	2088.471	1414.738	2492.812	342.495	2498.178	-35.267
3800	835.744	2110.745	1432.762	2576.333	341.169	2556.445	-35.140
3900	836.746	2132.467	1450.426	2659.958	339.590	2614.716	-35.019
4000	837.678	2153.663	1467.743	2743.680	337.744	2673.136	-34.907
4100	838.546	2174.358	1484.726	2827.491	335.603	2731.547	-34.800
4200	839.356	2194.575	1501.388	2911.387	333.188	2790.008	-34.698
4300	840.113	2214.334	1517.739	2995.361	330.488	2848.459	-34.601
4400	840.820	2233.656	1533.791	3079.408	327.511	2907.049	-34.510
4500	841.483	2252.560	1549.554	3163.523	324.267	2965.755	-34.425
4600	842.105	2271.061	1565.039	3247.703	320.716	3024.539	-34.344
4700	842.690	2289.178	1580.254	3331.943	316.868	3083.315	-34.266
4800	843.239	2306.925	1595.209	3416.240	312.761	3142.258	-34.194
4900	843.756	2324.318	1609.912	3500.590	308.337	3201.186	-34.124
5000	844.244	2341.369	1624.371	3584.990	303.670	3260.355	-34.060

3.110. 7H-Benzo[hi]chrysene



Other names: Naphthobenzanthrene

Formula: C₂₁H₁₄

Mass: 266.336 g/mol

CAS Number: 216-53-5

Point Group: C_s

Length: 13.85 Å

Width: 9.187 Å

Breadth: 4.176 Å

L/B Ratio: 1.507

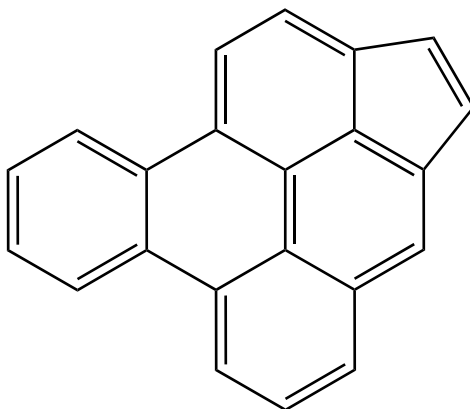
Cartesian coordinates:

C	-2.1876	2.5303	0.0000	C	0.8692	0.2823	0.0000	H	-5.1131	-1.3355	0.0000
C	-3.5944	2.4250	0.0000	C	0.0831	1.5506	0.0000	H	-3.7068	-3.3885	0.0000
C	-4.1969	1.1960	0.0000	C	2.3001	0.3654	0.0000	H	-1.2386	-3.2211	0.0000
C	-2.0016	0.1155	0.0000	C	3.0627	-0.8212	0.0000	H	3.0043	-2.9954	0.0000
C	-3.4092	0.0145	0.0000	C	4.4815	-0.7549	0.0000	H	0.5254	-3.1110	0.0000
C	-4.0195	-1.2677	0.0000	C	5.1179	0.4563	0.0000	H	0.3748	2.1512	0.8884
C	-3.2446	-2.3958	0.0000	C	4.3626	1.6497	0.0000	H	0.3748	2.1512	-0.8884
C	-1.8381	-2.2982	0.0000	C	2.9943	1.6077	0.0000	H	5.0540	-1.6895	0.0000
C	-1.2090	-1.0713	0.0000	C	-1.3987	1.4026	0.0000	H	6.2111	0.5141	0.0000
C	2.4026	-2.0794	0.0000	H	-1.7268	3.5245	0.0000	H	4.8871	2.6110	0.0000
C	1.0407	-2.1383	0.0000	H	-4.1956	3.3401	0.0000	H	2.4276	2.5463	0.0000
C	0.2514	-0.9541	0.0000	H	-5.2888	1.1052	0.0000				

Table 3.110: Table of thermodynamic data as a function of temperature for 7H-Benzo[hi]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-40.842	329.910	329.910	∞
100	90.596	329.394	678.661	-34.927	354.070	393.639	-205.612
200	174.407	416.414	525.886	-21.894	341.398	438.237	-114.453
250	223.815	460.590	508.390	-11.950	335.355	463.146	-96.767
298.15	272.512	504.178	504.178	0.000	329.910	488.264	-85.540
300	274.369	505.869	504.183	0.506	329.709	489.246	-85.183
350	323.409	551.879	507.705	15.461	324.630	516.247	-77.044
400	369.180	598.095	516.116	32.792	320.170	543.926	-71.028
450	410.846	644.026	527.781	52.310	316.273	572.133	-66.410
500	448.241	689.285	541.675	73.805	312.876	600.764	-62.760
600	511.276	776.803	573.632	121.903	307.332	658.890	-57.360
700	561.463	859.528	608.625	175.632	303.263	717.829	-53.564
800	601.971	937.238	644.896	233.873	300.492	777.247	-50.748
900	635.169	1010.119	681.471	295.784	298.849	836.940	-48.574
1000	662.725	1078.511	717.791	360.720	298.175	896.773	-46.842
1100	685.825	1142.790	753.536	428.180	298.288	956.640	-45.426
1200	705.343	1203.325	788.521	497.765	299.056	1016.453	-44.244
1300	721.942	1260.456	822.647	569.152	300.317	1076.191	-43.241
1400	736.141	1314.490	855.866	642.074	301.951	1135.820	-42.377
1500	748.353	1365.706	888.163	716.314	303.881	1195.322	-41.624
1600	758.909	1414.348	919.543	791.690	305.994	1254.682	-40.960
1700	768.078	1460.639	950.021	868.049	308.224	1313.886	-40.370
1800	776.079	1504.772	979.624	945.266	310.506	1373.008	-39.843
1900	783.092	1546.925	1008.381	1023.232	312.809	1431.961	-39.367
2000	789.266	1587.252	1036.324	1101.857	315.085	1490.814	-38.935
2100	794.723	1625.895	1063.485	1181.062	317.269	1549.543	-38.542
2200	799.566	1662.980	1089.898	1260.781	319.358	1608.175	-38.182
2300	803.880	1698.619	1115.594	1340.957	321.344	1666.710	-37.851
2400	807.737	1732.915	1140.606	1421.542	323.172	1725.127	-37.546
2500	811.197	1765.960	1164.963	1502.492	324.846	1783.559	-37.265
2600	814.311	1797.837	1188.695	1583.770	326.339	1841.836	-37.002
2700	817.123	1828.623	1211.829	1665.344	327.651	1900.114	-36.759
2800	819.669	1858.387	1234.392	1747.185	328.761	1958.367	-36.533
2900	821.980	1887.191	1256.408	1829.270	329.646	2016.540	-36.321
3000	824.085	1915.094	1277.902	1911.575	330.337	2074.707	-36.123
3100	826.007	1942.147	1298.895	1994.081	330.775	2132.796	-35.937
3200	827.765	1968.400	1319.409	2076.771	330.991	2190.931	-35.763
3300	829.378	1993.897	1339.464	2159.629	330.970	2249.093	-35.599
3400	830.860	2018.678	1359.078	2242.642	330.690	2307.194	-35.445
3500	832.226	2042.783	1378.269	2325.797	330.153	2365.292	-35.299
3600	833.487	2066.245	1397.055	2409.083	329.376	2423.474	-35.163
3700	834.653	2089.098	1415.452	2492.491	328.336	2481.699	-35.035
3800	835.733	2111.371	1433.474	2576.011	327.009	2539.904	-34.913
3900	836.736	2133.093	1451.135	2659.635	325.429	2598.111	-34.797
4000	837.669	2154.289	1468.450	2743.356	323.582	2656.469	-34.689
4100	838.538	2174.984	1485.431	2827.167	321.440	2714.818	-34.586
4200	839.348	2195.201	1502.091	2911.062	319.025	2773.216	-34.489
4300	840.105	2214.960	1518.440	2995.035	316.324	2831.604	-34.396
4400	840.813	2234.282	1534.491	3079.081	313.346	2890.132	-34.310
4500	841.476	2253.185	1550.252	3163.196	310.101	2948.776	-34.228
4600	842.098	2271.686	1565.735	3247.375	306.549	3007.497	-34.150
4700	842.683	2289.803	1580.949	3331.614	302.700	3066.210	-34.076
4800	843.232	2307.550	1595.902	3415.910	298.593	3125.091	-34.007
4900	843.750	2324.942	1610.604	3500.260	294.168	3183.956	-33.941
5000	844.238	2341.993	1625.062	3584.659	289.500	3243.063	-33.879

3.111. Benzo[*l*]cyclopenta[*cd*]pyrene



Other names: Benzo[*e*]cyclopenta[*jk*]pyrene

Formula: C₂₂H₁₂

Mass: 276.331 g/mol

CAS Number: 113779-16-1

Point Group: C_s

Length: 12.83 Å

Width: 10.43 Å

Breadth: 3.887 Å

L/B Ratio: 1.231

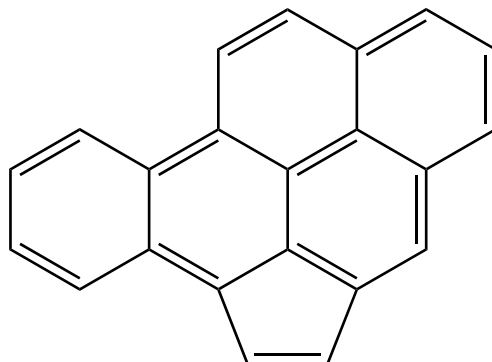
Cartesian coordinates:

C	-3.5246	-0.5909	0.0000	C	2.4529	1.9120	0.0000	H	1.9125	4.0062	0.0000
C	-2.1523	-0.2959	0.0000	C	1.9204	0.6057	0.0000	H	-0.5423	3.5308	0.0000
C	-1.7489	1.0573	0.0000	C	1.2070	-2.0550	0.0000	H	3.3597	-2.5027	0.0000
C	-2.7187	2.0703	0.0000	C	2.6161	-1.6986	0.0000	H	-2.6013	-2.9955	0.0000
C	-4.0658	1.7568	0.0000	C	2.9661	-0.3882	0.0000	H	-0.8549	-4.7725	0.0000
C	-4.4693	0.4198	0.0000	C	-1.5333	-2.7289	0.0000	H	1.5521	-4.1930	0.0000
C	-0.3343	1.3993	0.0000	C	-0.5507	-3.7202	0.0000	H	-2.3747	3.1164	0.0000
C	0.5727	0.3185	0.0000	C	0.7977	-3.3980	0.0000	H	-4.8162	2.5539	0.0000
C	0.1987	-1.0609	0.0000	C	4.2136	0.3994	0.0000	H	-5.5359	0.1727	0.0000
C	-1.1743	-1.3832	0.0000	C	3.9159	1.7308	0.0000	H	-3.8327	-1.6482	0.0000
C	0.1789	2.6988	0.0000	H	5.2042	-0.0507	0.0000				
C	1.5608	2.9700	0.0000	H	4.6211	2.5595	0.0000				

Table 3.111: Table of thermodynamic data as a function of temperature for Benzo[*l*]cyclopenta[*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-39.569	414.164	414.164	∞
100	84.394	316.822	658.369	-34.155	434.619	465.467	-243.130
200	170.717	400.244	508.377	-21.626	423.811	500.617	-130.745
250	221.183	443.719	491.071	-11.838	418.711	520.409	-108.731
298.15	270.412	486.896	486.896	0.000	414.164	540.419	-94.677
300	272.280	488.575	486.901	0.502	413.996	541.201	-94.230
350	321.400	534.274	490.398	15.356	409.794	562.744	-83.983
400	366.925	580.208	498.754	32.582	406.133	584.843	-76.371
450	408.135	625.848	510.345	51.977	402.946	607.376	-70.501
500	444.940	670.793	524.150	73.321	400.163	630.260	-65.841
600	506.570	757.588	555.887	121.021	395.572	676.732	-58.914
700	555.199	839.472	590.611	174.202	392.120	723.885	-54.016
800	594.108	916.241	626.569	231.737	389.675	771.450	-50.369
900	625.745	988.105	662.791	292.783	388.106	819.263	-47.548
1000	651.827	1055.427	698.725	356.702	387.295	867.219	-45.298
1100	673.571	1118.603	734.054	423.004	387.095	915.233	-43.460
1200	691.860	1178.018	768.600	491.301	387.403	963.228	-41.927
1300	707.359	1234.025	802.269	561.283	388.080	1011.190	-40.629
1400	720.579	1286.942	835.016	632.697	389.031	1059.092	-39.514
1500	731.922	1337.054	866.830	705.336	390.194	1106.921	-38.546
1600	741.708	1384.611	897.717	779.029	391.471	1154.660	-37.695
1700	750.195	1429.837	927.699	853.634	392.808	1202.298	-36.941
1800	757.592	1472.931	956.802	929.032	394.148	1249.908	-36.271
1900	764.069	1514.070	985.058	1005.122	395.468	1297.402	-35.667
2000	769.765	1553.409	1012.499	1081.820	396.727	1344.849	-35.123
2100	774.797	1591.090	1039.160	1159.053	397.867	1392.224	-34.629
2200	779.259	1627.239	1065.075	1236.760	398.886	1439.550	-34.179
2300	783.232	1661.968	1090.277	1314.889	399.782	1486.832	-33.766
2400	786.782	1695.378	1114.798	1393.393	400.500	1534.039	-33.387
2500	789.966	1727.562	1138.669	1472.233	401.050	1581.311	-33.039
2600	792.830	1758.602	1161.919	1551.375	401.405	1628.470	-32.716
2700	795.415	1788.573	1184.576	1630.790	401.567	1675.679	-32.417
2800	797.755	1817.543	1206.668	1710.450	401.518	1722.902	-32.140
2900	799.880	1845.575	1228.219	1790.333	401.233	1770.088	-31.882
3000	801.813	1872.725	1249.252	1870.420	400.749	1817.310	-31.642
3100	803.579	1899.046	1269.791	1950.691	400.004	1864.488	-31.416
3200	805.193	1924.584	1289.856	2031.130	399.032	1911.755	-31.206
3300	806.674	1949.384	1309.468	2111.725	397.818	1959.087	-31.009
3400	808.035	1973.486	1328.645	2192.461	396.341	2006.389	-30.824
3500	809.289	1996.928	1347.405	2273.328	394.604	2053.724	-30.650
3600	810.447	2019.743	1365.766	2354.316	392.625	2101.184	-30.487
3700	811.517	2041.963	1383.743	2435.415	390.380	2148.714	-30.334
3800	812.508	2063.618	1401.350	2516.617	387.848	2196.261	-30.189
3900	813.429	2084.735	1418.603	2597.914	385.062	2243.836	-30.052
4000	814.284	2105.340	1435.515	2679.300	382.008	2291.599	-29.925
4100	815.081	2125.457	1452.099	2760.769	378.658	2339.381	-29.803
4200	815.824	2145.107	1468.366	2842.315	375.036	2387.242	-29.689
4300	816.518	2164.312	1484.328	2923.932	371.130	2435.119	-29.580
4400	817.168	2183.091	1499.997	3005.617	366.946	2483.165	-29.478
4500	817.776	2201.462	1515.381	3087.364	362.498	2531.353	-29.383
4600	818.347	2219.442	1530.492	3169.171	357.742	2579.651	-29.292
4700	818.883	2237.048	1545.339	3251.033	352.692	2627.963	-29.206
4800	819.387	2254.293	1559.930	3332.946	347.384	2676.472	-29.125
4900	819.862	2271.193	1574.273	3414.909	341.759	2724.984	-29.048
5000	820.309	2287.761	1588.378	3496.918	335.891	2773.764	-28.977

3.112. Indeno[5,6,7,1-*defg*]chrysene



Formula: $C_{22}H_{12}$
Mass: 276.331 g/mol
CAS Number: 181270-04-2
Point Group: C_s

Length: 13.76 Å
Width: 10.30 Å
Breadth: 3.885 Å
L/B Ratio: 1.336

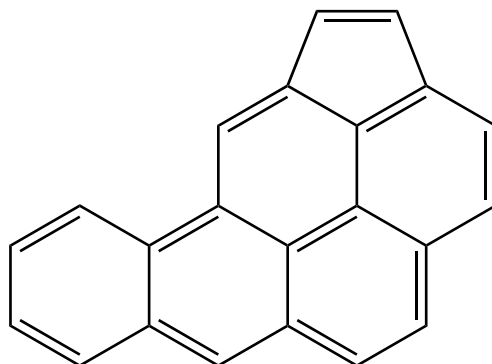
Cartesian coordinates:

C	0.0472	2.5321	0.0000	C	0.7405	-2.3359	0.0000	H	2.7713	-3.0355	0.0000
C	-0.5124	1.2128	0.0000	C	-2.8662	1.9666	0.0000	H	-2.4809	2.9983	0.0000
C	0.3927	0.1512	0.0000	C	-4.2107	1.7052	0.0000	H	-4.9356	2.5256	0.0000
C	1.8078	0.3101	0.0000	C	-4.6775	0.3726	0.0000	H	-5.7562	0.1852	0.0000
C	2.3222	1.6198	0.0000	C	-3.7908	-0.6720	0.0000	H	-4.1433	-1.7098	0.0000
C	1.3967	2.7212	0.0000	C	3.7189	1.7847	0.0000	H	4.7117	-1.4807	0.0000
C	-0.1024	-1.1547	0.0000	C	4.5451	0.6750	0.0000	H	5.6321	0.8112	0.0000
C	-1.4468	-1.4894	0.0000	C	4.0260	-0.6256	0.0000	H	4.1444	2.7944	0.0000
C	-2.3935	-0.4317	0.0000	C	-0.2186	-3.4558	0.0000	H	1.8132	3.7352	0.0000
C	-1.9176	0.9116	0.0000	C	-1.4919	-2.9607	0.0000	H	-0.6583	3.3771	0.0000
C	2.6513	-0.8368	0.0000	H	-2.4179	-3.5328	0.0000				
C	2.0842	-2.1824	0.0000	H	0.0795	-4.5018	0.0000				

Table 3.112: Table of thermodynamic data as a function of temperature for Indeno[5,6,7,1-defg]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-39.717	425.129	425.129	∞
100	84.790	316.022	659.305	-34.328	445.410	476.339	-248.809
200	171.698	399.960	508.572	-21.722	434.681	511.544	-133.599
250	222.171	443.657	491.194	-11.884	429.631	531.343	-111.016
298.15	271.336	487.003	487.003	0.000	425.129	551.353	-96.593
300	273.201	488.687	487.008	0.504	424.963	552.135	-96.133
350	322.226	534.521	490.516	15.402	420.805	573.668	-85.614
400	367.653	580.559	498.895	32.666	417.183	595.752	-77.796
450	408.775	626.280	510.514	52.095	414.030	618.266	-71.765
500	445.506	671.288	524.348	73.470	411.277	641.126	-66.977
600	507.025	758.176	556.143	121.220	406.737	687.544	-59.855
700	555.582	840.124	590.919	174.443	403.326	734.635	-54.818
800	594.442	916.941	626.924	232.014	400.917	782.132	-51.067
900	626.044	988.843	663.186	293.091	399.379	829.872	-48.164
1000	652.099	1056.194	699.156	357.038	398.597	877.753	-45.848
1100	673.821	1119.395	734.517	423.366	398.423	925.689	-43.956
1200	692.090	1178.831	769.091	491.688	398.754	973.604	-42.379
1300	707.571	1234.855	802.785	561.691	399.454	1021.484	-41.043
1400	720.774	1287.788	835.555	633.126	400.425	1069.303	-39.895
1500	732.103	1337.912	867.390	705.784	401.607	1117.046	-38.898
1600	741.876	1385.481	898.297	779.495	402.901	1164.699	-38.023
1700	750.350	1430.717	928.296	854.116	404.255	1212.249	-37.247
1800	757.736	1473.820	957.415	929.528	405.609	1259.771	-36.557
1900	764.202	1514.965	985.685	1005.632	406.943	1307.176	-35.936
2000	769.890	1554.312	1013.140	1082.343	408.216	1354.533	-35.376
2100	774.913	1591.999	1039.814	1159.588	409.367	1401.817	-34.868
2200	779.367	1628.152	1065.740	1237.307	410.397	1449.052	-34.404
2300	783.333	1662.886	1090.953	1315.445	411.304	1496.242	-33.980
2400	786.877	1696.300	1115.484	1393.959	412.032	1543.357	-33.590
2500	790.055	1728.488	1139.365	1472.809	412.591	1590.537	-33.232
2600	792.913	1759.531	1162.624	1551.959	412.954	1637.603	-32.899
2700	795.493	1789.505	1185.290	1631.382	413.125	1684.719	-32.592
2800	797.829	1818.478	1207.389	1711.050	413.083	1731.849	-32.307
2900	799.949	1846.513	1228.947	1790.941	412.805	1778.941	-32.042
3000	801.879	1873.665	1249.987	1871.033	412.328	1826.069	-31.794
3100	803.640	1899.988	1270.533	1951.311	411.590	1873.153	-31.562
3200	805.252	1925.528	1290.604	2031.756	410.623	1920.325	-31.345
3300	806.730	1950.330	1310.222	2112.357	409.415	1967.563	-31.143
3400	808.088	1974.434	1329.405	2193.098	407.943	2014.770	-30.953
3500	809.339	1997.877	1348.171	2273.971	406.212	2062.010	-30.773
3600	810.494	2020.693	1366.536	2354.963	404.238	2109.375	-30.606
3700	811.562	2042.914	1384.518	2436.067	401.997	2156.810	-30.448
3800	812.551	2064.570	1402.130	2517.273	399.470	2204.263	-30.299
3900	813.470	2085.689	1419.388	2598.574	396.687	2251.742	-30.158
4000	814.323	2106.295	1436.304	2679.965	393.637	2299.409	-30.027
4100	815.118	2126.413	1452.891	2761.437	390.292	2347.096	-29.902
4200	815.860	2146.064	1469.163	2842.987	386.673	2394.861	-29.784
4300	816.553	2165.270	1485.129	2924.608	382.770	2442.643	-29.672
4400	817.201	2184.050	1500.801	3006.296	378.590	2490.592	-29.566
4500	817.808	2202.421	1516.189	3088.046	374.145	2538.685	-29.468
4600	818.377	2220.402	1531.303	3169.856	369.393	2586.887	-29.374
4700	818.912	2238.008	1546.153	3251.721	364.346	2635.103	-29.285
4800	819.415	2255.254	1560.747	3333.637	359.040	2683.516	-29.202
4900	819.889	2272.155	1575.093	3415.603	353.418	2731.932	-29.122
5000	820.335	2288.723	1589.201	3497.614	347.553	2780.616	-29.048

3.113. Benzo[def]cyclopenta[qr]chrysene



Formula: $C_{22}H_{12}$
Mass: 276.331 g/mol
CAS Number: 153043-82-4
Point Group: C_s

Length: 13.73 Å
Width: 10.30 Å
Breadth: 3.889 Å
L/B Ratio: 1.333

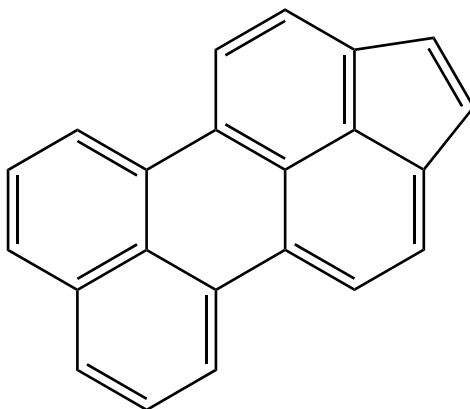
Cartesian coordinates:

C	-4.2450	-0.7713	0.0000	C	1.2776	1.9470	0.0000	H	4.2330	-2.3962	0.0000
C	-2.8248	-0.7029	0.0000	C	-0.0826	1.9181	0.0000	H	5.2782	-0.1485	0.0000
C	-2.1970	0.5631	0.0000	C	2.2022	-1.6888	0.0000	H	-0.6964	2.8312	0.0000
C	-3.0052	1.7305	0.0000	C	3.5860	-1.5115	0.0000	H	-2.5755	-2.8662	0.0000
C	-4.3710	1.6376	0.0000	C	4.1870	-0.2340	0.0000	H	-0.3469	-3.9958	0.0000
C	-4.9982	0.3718	0.0000	C	3.3845	0.8911	0.0000	H	2.1217	-3.8735	0.0000
C	-0.7667	0.6435	0.0000	C	0.1621	-3.0246	0.0000	H	-2.4995	2.7084	0.0000
C	-0.0491	-0.5630	0.0000	C	1.5139	-2.9618	0.0000	H	-4.9896	2.5409	0.0000
C	-0.6826	-1.8423	0.0000	C	3.5638	2.3543	0.0000	H	-6.0918	0.3180	0.0000
C	-2.0565	-1.8998	0.0000	C	2.3438	2.9665	0.0000	H	-4.7261	-1.7562	0.0000
C	1.3755	-0.5396	0.0000	H	2.1480	4.0367	0.0000				
C	1.9852	0.6962	0.0000	H	4.5386	2.8378	0.0000				

Table 3.113: Table of thermodynamic data as a function of temperature for Benzo[def]cyclopenta[qr]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-39.445	427.676	427.676	∞
100	83.615	315.641	656.684	-34.104	448.182	479.148	-250.276
200	170.510	398.677	506.819	-21.628	437.322	514.442	-134.356
250	221.229	442.135	489.510	-11.844	432.219	534.312	-111.636
298.15	270.575	485.332	485.332	0.000	427.676	554.398	-97.126
300	272.445	487.012	485.337	0.502	427.509	555.183	-96.664
350	321.591	532.739	488.837	15.366	423.316	576.803	-86.081
400	367.097	578.698	497.197	32.600	419.665	598.978	-78.217
450	408.275	624.357	508.794	52.003	416.485	621.587	-72.150
500	445.051	669.314	522.606	73.354	413.708	644.544	-67.334
600	506.642	756.126	554.355	121.062	409.126	691.164	-60.170
700	555.261	838.020	589.090	174.251	405.681	738.463	-55.104
800	594.174	914.797	625.058	231.792	403.242	786.172	-51.331
900	625.820	986.670	661.288	292.844	401.680	834.129	-48.411
1000	651.913	1054.000	697.229	356.771	400.878	882.228	-46.082
1100	673.664	1117.185	732.564	423.082	400.687	930.384	-44.179
1200	691.957	1176.608	767.117	491.389	401.003	978.520	-42.593
1300	707.458	1232.623	800.791	561.381	401.691	1026.624	-41.249
1400	720.678	1285.548	833.544	632.805	402.651	1074.666	-40.095
1500	732.019	1335.666	865.363	705.454	403.824	1122.634	-39.093
1600	741.803	1383.229	896.256	779.157	405.111	1170.511	-38.212
1700	750.286	1428.461	926.243	853.771	406.457	1218.287	-37.433
1800	757.679	1471.560	955.351	929.178	407.806	1266.035	-36.739
1900	764.152	1512.703	983.610	1005.276	409.134	1313.665	-36.114
2000	769.845	1552.047	1011.056	1081.982	410.402	1361.249	-35.551
2100	774.872	1589.732	1037.721	1159.223	411.549	1408.760	-35.040
2200	779.331	1625.884	1063.639	1236.938	412.576	1456.221	-34.574
2300	783.300	1660.616	1088.845	1315.073	413.479	1503.638	-34.148
2400	786.847	1694.029	1113.369	1393.584	414.204	1550.981	-33.756
2500	790.027	1726.215	1137.243	1472.430	414.760	1598.387	-33.396
2600	792.888	1757.257	1160.497	1551.578	415.121	1645.681	-33.061
2700	795.470	1787.231	1183.157	1630.998	415.289	1693.024	-32.753
2800	797.807	1816.203	1205.251	1710.664	415.244	1740.381	-32.467
2900	799.929	1844.237	1226.805	1790.553	414.965	1787.702	-32.199
3000	801.860	1871.388	1247.841	1870.644	414.486	1835.057	-31.951
3100	803.623	1897.710	1268.382	1950.919	413.745	1882.369	-31.717
3200	805.236	1923.250	1288.449	2031.363	412.778	1929.769	-31.500
3300	806.715	1948.052	1308.063	2111.962	411.568	1977.234	-31.296
3400	808.074	1972.155	1327.243	2192.702	410.094	2024.669	-31.105
3500	809.326	1995.597	1346.005	2273.573	408.361	2072.137	-30.924
3600	810.481	2018.413	1364.368	2354.564	406.386	2119.730	-30.756
3700	811.550	2040.634	1382.346	2435.666	404.145	2167.393	-30.597
3800	812.540	2062.290	1399.956	2516.872	401.616	2215.074	-30.448
3900	813.459	2083.408	1417.210	2598.172	398.832	2262.781	-30.306
4000	814.313	2104.014	1434.124	2679.561	395.781	2310.676	-30.174
4100	815.109	2124.132	1450.709	2761.033	392.435	2358.591	-30.048
4200	815.851	2143.783	1466.978	2842.581	388.815	2406.584	-29.930
4300	816.544	2162.988	1482.942	2924.201	384.912	2454.594	-29.817
4400	817.193	2181.768	1498.611	3005.889	380.731	2502.772	-29.711
4500	817.800	2200.139	1513.998	3087.638	376.285	2551.092	-29.612
4600	818.370	2218.120	1529.110	3169.447	371.532	2599.523	-29.518
4700	818.905	2235.726	1543.958	3251.311	366.484	2647.967	-29.428
4800	819.408	2252.972	1558.550	3333.227	361.177	2696.608	-29.344
4900	819.882	2269.873	1572.895	3415.192	355.554	2745.252	-29.264
5000	820.329	2286.441	1587.000	3497.203	349.689	2794.164	-29.190

3.114. Cyclopenta[*cd*]perylene



Other names: Aceperylene
Formula: C₂₂H₁₂
Mass: 276.331 g/mol
CAS Number: 189-01-5
Point Group: C_{2v}

Length: 12.86 Å
Width: 9.184 Å
Breadth: 3.887 Å
L/B Ratio: 1.400

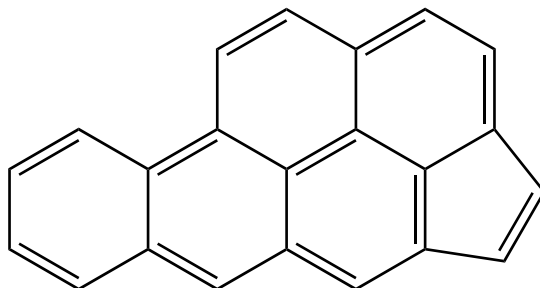
Cartesian coordinates:

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C	0.3217	-1.2577	0.0000	C	-3.2759	-0.1070	0.0000	H	0.4235	3.4030	0.0000
C	0.9265	0.0303	0.0000	C	-4.0213	1.1029	0.0000	H	0.6448	-3.3681	0.0000
C	0.2390	1.2760	0.0000	C	-3.3803	2.3131	0.0000	H	3.1391	-3.2305	0.0000
C	-1.2189	1.2172	0.0000	C	-1.9724	2.3713	0.0000	H	-1.4555	3.3436	0.0000
C	-1.8653	-0.0609	0.0000	C	-1.8135	-2.4949	0.0000	H	-3.9520	3.2470	0.0000
C	0.9743	2.4495	0.0000	C	-3.2222	-2.5287	0.0000	H	-5.1160	1.0495	0.0000
C	2.3960	2.4687	0.0000	C	-3.9408	-1.3629	0.0000	H	-5.0367	-1.3810	0.0000
C	3.0735	1.2764	0.0000	C	4.5220	-0.5350	0.0000	H	-3.7317	-3.4979	0.0000
C	2.3060	0.0753	0.0000	C	4.4774	0.8288	0.0000	H	-1.2342	-3.4315	0.0000
C	1.1321	-2.3807	0.0000	H	5.4111	-1.1620	0.0000				
C	2.5520	-2.3070	0.0000	H	5.3237	1.5127	0.0000				

Table 3.114: Table of thermodynamic data as a function of temperature for Cyclopenta[cd]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-39.555	439.722	439.722	∞
100	84.371	311.781	653.101	-34.132	460.200	491.553	-256.755
200	170.581	395.120	503.203	-21.617	449.380	527.211	-137.690
250	221.087	438.569	485.905	-11.834	444.274	547.259	-114.341
298.15	270.331	481.731	481.731	0.000	439.722	567.518	-99.425
300	272.200	483.409	481.736	0.502	439.554	568.309	-98.949
350	321.324	529.096	485.232	15.352	435.349	590.111	-88.067
400	366.854	575.021	493.586	32.574	431.684	612.469	-79.979
450	408.073	620.653	505.174	51.966	428.494	635.262	-73.738
500	444.891	665.592	518.976	73.308	425.708	658.405	-68.782
600	506.545	752.380	550.708	121.003	421.113	705.398	-61.409
700	555.195	834.262	585.428	174.184	417.660	753.072	-56.194
800	594.119	911.032	621.383	231.719	415.215	801.158	-52.309
900	625.766	982.898	657.603	292.766	413.648	849.491	-49.302
1000	651.855	1050.222	693.534	356.687	412.839	897.968	-46.904
1100	673.602	1113.401	728.862	422.992	412.642	946.502	-44.945
1200	691.893	1172.818	763.408	491.293	412.953	995.017	-43.311
1300	707.392	1228.828	797.076	561.278	413.634	1043.500	-41.927
1400	720.611	1281.748	829.823	632.695	414.587	1091.921	-40.739
1500	731.953	1331.861	861.636	705.338	415.754	1140.270	-39.707
1600	741.738	1379.421	892.524	779.034	417.034	1188.527	-38.801
1700	750.224	1424.649	922.507	853.642	418.374	1236.685	-37.998
1800	757.619	1467.745	951.610	929.042	419.717	1284.814	-37.284
1900	764.095	1508.884	979.866	1005.135	421.039	1332.826	-36.641
2000	769.790	1548.225	1007.307	1081.835	422.302	1380.791	-36.062
2100	774.820	1585.907	1033.969	1159.071	423.443	1428.685	-35.536
2200	779.281	1622.057	1059.884	1236.780	424.465	1476.529	-35.057
2300	783.253	1656.787	1085.086	1314.911	425.363	1524.329	-34.618
2400	786.802	1690.198	1109.608	1393.417	426.083	1572.054	-34.214
2500	789.984	1722.383	1133.479	1472.259	426.635	1619.844	-33.844
2600	792.847	1753.423	1156.730	1551.403	426.991	1667.521	-33.500
2700	795.432	1783.395	1179.388	1630.819	427.155	1715.248	-33.183
2800	797.771	1812.366	1201.479	1710.481	427.107	1762.988	-32.888
2900	799.894	1840.398	1223.030	1790.366	426.824	1810.693	-32.613
3000	801.827	1867.549	1244.064	1870.454	426.342	1858.431	-32.357
3100	803.592	1893.870	1264.603	1950.726	425.598	1906.128	-32.117
3200	805.206	1919.409	1284.669	2031.167	424.627	1953.912	-31.894
3300	806.686	1944.209	1304.281	2111.763	423.415	2001.761	-31.685
3400	808.047	1968.312	1323.459	2192.500	421.939	2049.581	-31.487
3500	809.300	1991.753	1342.219	2273.369	420.203	2097.433	-31.302
3600	810.457	2014.568	1360.580	2354.357	418.225	2145.410	-31.128
3700	811.526	2036.789	1378.557	2435.457	415.981	2193.458	-30.965
3800	812.518	2058.444	1396.165	2516.660	413.450	2241.523	-30.811
3900	813.437	2079.562	1413.419	2597.958	410.664	2289.615	-30.665
4000	814.293	2100.167	1430.331	2679.345	407.611	2337.895	-30.529
4100	815.089	2120.284	1446.915	2760.815	404.263	2386.195	-30.400
4200	815.832	2139.935	1463.182	2842.361	400.641	2434.573	-30.278
4300	816.526	2159.140	1479.145	2923.980	396.736	2482.967	-30.161
4400	817.175	2177.919	1494.813	3005.665	392.553	2531.530	-30.052
4500	817.783	2196.290	1510.198	3087.413	388.105	2580.235	-29.950
4600	818.354	2214.270	1525.309	3169.220	383.351	2629.051	-29.853
4700	818.889	2231.876	1540.156	3251.083	378.301	2677.880	-29.761
4800	819.393	2249.122	1554.747	3332.997	372.993	2726.906	-29.674
4900	819.868	2266.022	1569.091	3414.960	367.369	2775.935	-29.591
5000	820.315	2282.590	1583.196	3496.970	361.502	2825.233	-29.514

3.115. Indeno[1,7,6,5-*cdef*]chrysene



Formula: $C_{22}H_{12}$
Mass: 276.331 g/mol
CAS Number: 153043-81-3
Point Group: C_s

Length: 13.91 Å
Width: 9.574 Å
Breadth: 3.885 Å
L/B Ratio: 1.453

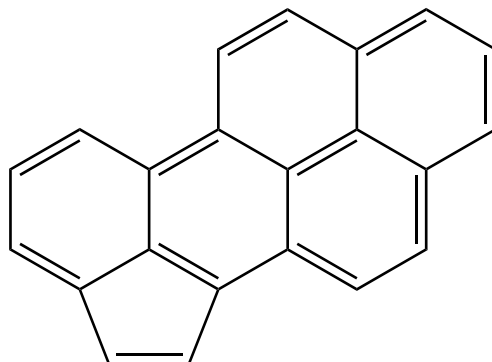
Cartesian coordinates:

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C	-3.6420	-0.0991	0.0000	C	-2.3030	0.3034	0.0000	H	-0.5066	-3.8984	0.0000
C	-3.9065	-1.4705	0.0000	C	-1.2286	-0.5694	0.0000	H	1.7976	-2.9498	0.0000
C	-2.8415	-2.3721	0.0000	C	2.6392	1.0799	0.0000	H	1.6672	3.0248	0.0000
C	-1.4939	-1.9524	0.0000	C	2.4838	-0.3239	0.0000	H	-0.7866	3.3803	0.0000
C	-0.3466	-2.8147	0.0000	C	3.6368	-1.1503	0.0000	H	3.4853	-2.2409	0.0000
C	0.9124	-2.2941	0.0000	C	4.8897	-0.5979	0.0000	H	5.7792	-1.2363	0.0000
C	1.1657	-0.8784	0.0000	C	5.0477	0.8061	0.0000	H	6.0578	1.2287	0.0000
C	1.5051	1.9395	0.0000	C	3.9512	1.6266	0.0000	H	4.0702	2.7163	0.0000
C	0.0794	-0.0049	0.0000	H	-3.8533	3.2738	0.0000				
C	0.2284	1.4251	0.0000	H	-5.5125	1.1744	0.0000				

Table 3.115: Table of thermodynamic data as a function of temperature for Indeno[1,7,6,5-*cdef*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-39.585	425.489	425.489	∞
100	84.076	316.526	658.570	-34.204	445.895	476.773	-249.035
200	171.018	399.887	508.294	-21.682	435.082	511.959	-133.707
250	221.774	443.463	490.944	-11.870	430.005	531.766	-111.104
298.15	271.134	486.757	486.757	0.000	425.489	551.786	-96.669
300	273.005	488.440	486.762	0.503	425.322	552.569	-96.209
350	322.149	534.254	490.268	15.395	421.158	574.115	-85.680
400	367.642	580.286	498.644	32.657	417.534	596.212	-77.856
450	408.798	626.008	510.261	52.086	414.382	618.740	-71.820
500	445.547	671.019	524.093	73.463	411.630	641.614	-67.028
600	507.081	757.916	555.886	121.218	407.095	688.058	-59.900
700	555.644	839.874	590.663	174.447	403.691	735.174	-54.858
800	594.509	916.699	626.669	232.024	401.288	782.696	-51.104
900	626.113	988.609	662.933	293.108	399.757	830.460	-48.198
1000	652.170	1055.968	698.905	357.063	398.982	878.364	-45.880
1100	673.891	1119.175	734.268	423.398	398.815	926.323	-43.986
1200	692.159	1178.617	768.846	491.726	399.153	974.259	-42.408
1300	707.638	1234.648	802.542	561.737	399.860	1022.160	-41.070
1400	720.839	1287.585	835.315	633.178	400.837	1069.999	-39.921
1500	732.164	1337.714	867.152	705.842	402.025	1117.763	-38.923
1600	741.934	1385.286	898.062	779.559	403.326	1165.435	-38.047
1700	750.406	1430.526	928.063	854.186	404.685	1213.005	-37.270
1800	757.788	1473.631	957.185	929.604	406.045	1260.546	-36.579
1900	764.252	1514.780	985.457	1005.713	407.384	1307.969	-35.958
2000	769.936	1554.128	1012.914	1082.428	408.661	1355.344	-35.397
2100	774.956	1591.818	1039.590	1159.678	409.817	1402.647	-34.888
2200	779.408	1627.973	1065.519	1237.400	410.851	1449.900	-34.424
2300	783.372	1662.709	1090.733	1315.543	411.762	1497.108	-34.000
2400	786.913	1696.125	1115.266	1394.061	412.494	1544.241	-33.609
2500	790.089	1728.314	1139.148	1472.914	413.057	1591.437	-33.251
2600	792.945	1759.358	1162.409	1552.068	413.423	1638.522	-32.918
2700	795.524	1789.333	1185.077	1631.493	413.596	1685.655	-32.610
2800	797.857	1818.308	1207.177	1711.164	413.557	1732.801	-32.325
2900	799.976	1846.343	1228.737	1791.058	413.283	1779.911	-32.059
3000	801.905	1873.496	1249.779	1871.153	412.808	1827.055	-31.811
3100	803.665	1899.820	1270.325	1951.433	412.072	1874.156	-31.579
3200	805.275	1925.361	1290.398	2031.881	411.108	1921.345	-31.362
3300	806.752	1950.164	1310.017	2112.484	409.903	1968.600	-31.160
3400	808.109	1974.268	1329.201	2193.228	408.433	2015.824	-30.969
3500	809.359	1997.711	1347.968	2274.102	406.703	2063.080	-30.789
3600	810.513	2020.528	1366.335	2355.096	404.731	2110.461	-30.621
3700	811.580	2042.750	1384.317	2436.201	402.493	2157.913	-30.464
3800	812.568	2064.407	1401.931	2517.409	399.967	2205.382	-30.314
3900	813.486	2085.526	1419.189	2598.713	397.186	2252.878	-30.173
4000	814.339	2106.132	1436.106	2680.105	394.138	2300.561	-30.042
4100	815.134	2126.250	1452.694	2761.579	390.794	2348.264	-29.917
4200	815.874	2145.902	1468.966	2843.129	387.177	2396.045	-29.799
4300	816.567	2165.108	1484.933	2924.752	383.275	2443.843	-29.686
4400	817.214	2183.888	1500.606	3006.441	379.096	2491.809	-29.581
4500	817.821	2202.260	1515.995	3088.193	374.653	2539.917	-29.482
4600	818.390	2220.241	1531.110	3170.004	369.901	2588.136	-29.389
4700	818.924	2237.847	1545.960	3251.870	364.855	2636.368	-29.299
4800	819.426	2255.094	1560.555	3333.788	359.551	2684.797	-29.216
4900	819.900	2271.995	1574.902	3415.754	353.930	2733.229	-29.136
5000	820.345	2288.563	1589.010	3497.767	348.066	2781.929	-29.062

3.116. Indeno[1,7-*ab*]pyrene



Other names: Benzo[*def*]cyclopenta[*hi*]chrysene

Formula: C₂₂H₁₂

Mass: 276.331 g/mol

CAS Number: 196-77-0

Point Group: C_s

Length: 13.78 Å

Width: 9.227 Å

Breadth: 3.884 Å

L/B Ratio: 1.493

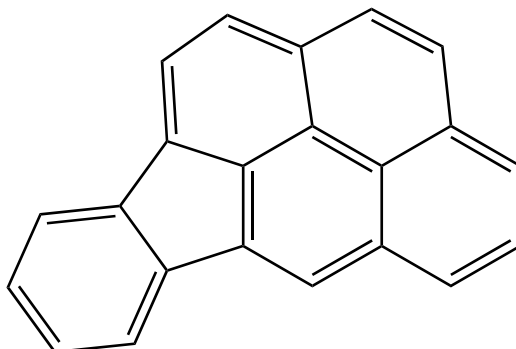
Cartesian coordinates:

C	0.4731	2.4209	0.0000	C	-4.4493	0.6108	0.0000	H	-4.6060	2.7684	0.0000
C	-0.1973	1.1584	0.0000	C	-3.5819	-0.4477	0.0000	H	-5.5342	0.4689	0.0000
C	0.5507	-0.0335	0.0000	C	2.7693	-1.1364	0.0000	H	-2.1576	3.1985	0.0000
C	1.9825	0.0449	0.0000	C	2.1090	-2.4225	0.0000	H	0.2607	-3.4894	0.0000
C	2.6232	1.3028	0.0000	C	0.7640	-2.5154	0.0000	H	2.7383	-3.3200	0.0000
C	1.8288	2.4948	0.0000	C	4.0289	1.3670	0.0000	H	4.7655	-1.9537	0.0000
C	-0.0699	-1.3369	0.0000	C	4.7798	0.2081	0.0000	H	5.8735	0.2639	0.0000
C	-1.4442	-1.3994	0.0000	C	4.1560	-1.0427	0.0000	H	4.5214	2.3461	0.0000
C	-2.1799	-0.1764	0.0000	C	-3.7006	-1.9149	0.0000	H	2.3409	3.4638	0.0000
C	-1.6279	1.0945	0.0000	C	-2.4549	-2.4683	0.0000	H	-0.1527	3.3249	0.0000
C	-2.5529	2.1738	0.0000	H	-4.6539	-2.4393	0.0000				
C	-3.9064	1.9253	0.0000	H	-2.2064	-3.5281	0.0000				

Table 3.116: Table of thermodynamic data as a function of temperature for Indeno[1,7-*ab*]pyrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-39.459	414.503	414.503	∞
100	83.658	315.173	656.514	-34.134	434.979	465.993	-243.405
200	170.694	398.341	506.534	-21.639	424.139	501.326	-130.930
250	221.330	441.831	489.218	-11.847	419.043	521.212	-108.899
298.15	270.609	485.040	485.040	0.000	414.503	541.313	-94.834
300	272.478	486.719	485.045	0.502	414.336	542.098	-94.386
350	321.583	532.448	488.544	15.366	410.144	563.733	-84.131
400	367.070	578.405	496.905	32.600	406.491	585.922	-76.512
450	408.242	624.060	508.502	52.001	403.311	608.546	-70.637
500	445.017	669.014	522.313	73.351	400.532	631.518	-65.973
600	506.614	755.819	554.060	121.055	395.947	678.168	-59.039
700	555.236	837.709	588.793	174.241	392.499	725.498	-54.136
800	594.150	914.484	624.759	231.780	390.058	773.238	-50.486
900	625.795	986.354	660.987	292.830	388.493	821.226	-47.662
1000	651.886	1053.681	696.926	356.755	387.688	869.357	-45.410
1100	673.636	1116.863	732.260	423.063	387.494	917.546	-43.570
1200	691.929	1176.284	766.811	491.367	387.808	965.714	-42.036
1300	707.430	1232.296	800.484	561.356	388.493	1013.850	-40.736
1400	720.650	1285.219	833.236	632.777	389.450	1061.925	-39.620
1500	731.992	1335.335	865.053	705.423	390.621	1109.926	-38.650
1600	741.776	1382.897	895.945	779.123	391.905	1157.836	-37.799
1700	750.261	1428.127	925.930	853.735	393.249	1205.645	-37.044
1800	757.655	1471.225	955.037	929.139	394.595	1253.426	-36.373
1900	764.129	1512.367	983.296	1005.235	395.921	1301.091	-35.769
2000	769.823	1551.709	1010.740	1081.939	397.187	1348.708	-35.224
2100	774.852	1589.393	1037.404	1159.178	398.331	1396.253	-34.729
2200	779.311	1625.544	1063.321	1236.890	399.356	1443.748	-34.278
2300	783.282	1660.275	1088.526	1315.024	400.257	1491.199	-33.865
2400	786.829	1693.688	1113.049	1393.533	400.980	1538.575	-33.486
2500	790.010	1725.874	1136.923	1472.377	401.535	1586.016	-33.137
2600	792.872	1756.915	1160.175	1551.524	401.894	1633.344	-32.814
2700	795.455	1786.888	1182.835	1630.943	402.060	1680.722	-32.515
2800	797.793	1815.859	1204.928	1710.607	402.014	1728.113	-32.238
2900	799.915	1843.893	1226.481	1790.494	401.733	1775.468	-31.979
3000	801.847	1871.044	1247.516	1870.584	401.253	1822.857	-31.738
3100	803.611	1897.366	1268.057	1950.858	400.511	1870.204	-31.512
3200	805.224	1922.905	1288.124	2031.301	399.542	1917.638	-31.302
3300	806.704	1947.706	1307.737	2111.898	398.332	1965.138	-31.105
3400	808.063	1971.809	1326.916	2192.638	396.857	2012.608	-30.919
3500	809.316	1995.251	1345.678	2273.507	395.123	2060.111	-30.745
3600	810.472	2018.067	1364.040	2354.497	393.147	2107.738	-30.582
3700	811.541	2040.288	1382.018	2435.599	390.904	2155.436	-30.429
3800	812.531	2061.943	1399.627	2516.803	388.374	2203.151	-30.284
3900	813.451	2083.061	1416.881	2598.103	385.590	2250.893	-30.147
4000	814.305	2103.667	1433.794	2679.491	382.538	2298.823	-30.019
4100	815.101	2123.784	1450.379	2760.962	379.191	2346.773	-29.898
4200	815.844	2143.435	1466.647	2842.509	375.571	2394.801	-29.783
4300	816.537	2162.640	1482.611	2924.129	371.666	2442.845	-29.674
4400	817.186	2181.420	1498.280	3005.815	367.485	2491.058	-29.572
4500	817.794	2199.791	1513.666	3087.565	363.038	2539.413	-29.476
4600	818.364	2217.772	1528.778	3169.373	358.284	2587.878	-29.386
4700	818.899	2235.377	1543.625	3251.236	353.236	2636.358	-29.299
4800	819.403	2252.623	1558.217	3333.152	347.929	2685.033	-29.219
4900	819.877	2269.524	1572.561	3415.116	342.305	2733.712	-29.141
5000	820.323	2286.092	1586.667	3497.126	336.439	2782.659	-29.070

3.117. Indeno[1,2,3-*cd*]pyrene



Other names: 1,10-(1,2-Phenylene)pyrene
 1,10-(*o*-Phenylene)pyrene
o-Phenylene-pyrene
 2,3-(*o*-Phenylene)pyrene
 2,3-Phenylene-pyrene

Formula: C₂₂H₁₂
Mass: 276.331 g/mol
CAS Number: 193-39-5
Point Group: C_s

Length: 13.74 Å
Width: 9.883 Å
Breadth: 3.885 Å
L/B Ratio: 1.390

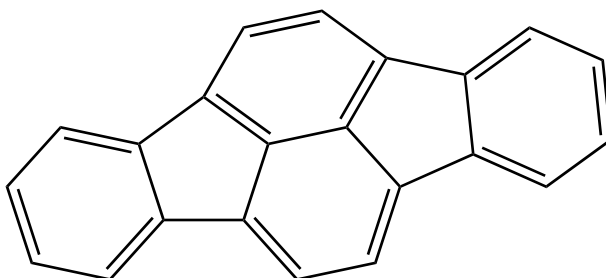
Cartesian coordinates:

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C	-4.6394	-1.4817	0.0000	C	2.4651	-2.6598	0.0000	H	-4.2958	1.9212	0.0000
C	-3.2959	-1.8787	0.0000	C	3.8122	-2.3097	0.0000	H	0.4542	4.1029	0.0000
C	-4.0132	0.8638	0.0000	C	4.2193	-0.9790	0.0000	H	-1.9283	3.4036	0.0000
C	-2.6861	0.4874	0.0000	C	-0.4003	0.3657	0.0000	H	4.6710	1.7039	0.0000
C	-2.3230	-0.9011	0.0000	C	-0.8557	-1.0070	0.0000	H	2.9504	3.4827	0.0000
C	-1.4571	1.2946	0.0000	C	0.0608	-2.0057	0.0000	H	2.1759	-3.7169	0.0000
C	0.2102	3.0345	0.0000	C	1.4757	-1.6709	0.0000	H	4.5699	-3.1010	0.0000
C	-1.1383	2.6456	0.0000	C	1.9016	-0.3180	0.0000	H	5.2861	-0.7292	0.0000
C	1.2578	2.1033	0.0000	C	0.9337	0.7293	0.0000	H	-0.2295	-3.0619	0.0000
C	3.6051	1.4475	0.0000	H	-6.0478	0.1442	0.0000				
C	2.6641	2.4251	0.0000	H	-5.4225	-2.2472	0.0000				

Table 3.117: Table of thermodynamic data as a function of temperature for Indeno[1,2,3-*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-39.158	371.002	371.002	∞
100	83.347	314.152	652.865	-33.871	391.740	422.856	-220.873
200	169.266	396.710	504.061	-21.470	380.806	458.319	-119.698
250	219.586	439.845	486.878	-11.758	375.630	478.295	-99.932
298.15	268.692	482.730	482.730	0.000	371.002	498.500	-87.333
300	270.556	484.398	482.735	0.499	370.831	499.289	-86.932
350	319.599	529.825	486.211	15.265	366.541	521.048	-77.761
400	365.104	575.517	494.519	32.399	362.789	543.375	-70.956
450	406.349	620.944	506.047	51.704	359.512	566.149	-65.715
500	443.231	665.704	519.781	72.961	356.641	589.282	-61.561
600	505.088	752.206	551.373	120.500	351.890	636.279	-55.392
700	553.978	833.881	585.957	173.547	348.303	683.981	-51.038
800	593.134	910.504	621.789	230.972	345.748	732.113	-47.801
900	624.983	982.266	657.899	291.931	344.093	780.504	-45.298
1000	651.240	1049.517	693.734	355.783	343.215	829.048	-43.304
1100	673.123	1112.644	728.977	422.034	342.963	877.656	-41.676
1200	691.520	1172.025	763.448	490.292	343.231	926.248	-40.318
1300	707.102	1228.008	797.051	560.244	343.880	974.811	-39.168
1400	720.386	1280.909	829.741	631.636	344.807	1023.316	-38.180
1500	731.778	1331.009	861.503	704.258	345.954	1071.749	-37.321
1600	741.603	1378.558	892.346	777.939	347.219	1120.093	-36.567
1700	750.119	1423.779	922.288	852.535	348.547	1168.337	-35.898
1800	757.538	1466.869	951.355	927.926	349.880	1216.553	-35.303
1900	764.032	1508.005	979.578	1004.012	351.196	1264.653	-34.767
2000	769.742	1547.343	1006.990	1080.707	352.452	1312.707	-34.284
2100	774.784	1585.023	1033.624	1157.938	353.590	1360.688	-33.845
2200	779.254	1621.171	1059.515	1235.644	354.608	1408.621	-33.444
2300	783.233	1655.900	1084.695	1313.772	355.504	1456.509	-33.078
2400	786.788	1689.311	1109.195	1392.277	356.223	1504.323	-32.740
2500	789.975	1721.495	1133.048	1471.118	356.774	1552.202	-32.431
2600	792.842	1752.535	1156.281	1550.261	357.129	1599.968	-32.143
2700	795.429	1782.506	1178.922	1629.677	357.293	1647.783	-31.878
2800	797.771	1811.477	1200.999	1709.339	357.245	1695.613	-31.631
2900	799.896	1839.510	1222.536	1789.224	356.962	1743.406	-31.401
3000	801.831	1866.661	1243.557	1869.312	356.479	1791.233	-31.188
3100	803.596	1892.982	1264.084	1949.584	355.736	1839.019	-30.987
3200	805.211	1918.521	1284.138	2030.026	354.766	1886.891	-30.800
3300	806.692	1943.321	1303.739	2110.622	353.554	1934.830	-30.625
3400	808.054	1967.424	1322.906	2191.360	352.078	1982.738	-30.460
3500	809.307	1990.866	1341.658	2272.229	350.343	2030.679	-30.306
3600	810.464	2013.681	1360.009	2353.219	348.366	2078.745	-30.161
3700	811.534	2035.902	1377.978	2434.319	346.123	2126.881	-30.026
3800	812.525	2057.557	1395.578	2515.523	343.593	2175.035	-29.897
3900	813.445	2078.675	1412.823	2596.822	340.808	2223.216	-29.776
4000	814.301	2099.281	1429.728	2678.210	337.755	2271.584	-29.663
4100	815.097	2119.398	1446.305	2759.680	334.408	2319.973	-29.556
4200	815.840	2139.049	1462.566	2841.227	330.787	2368.439	-29.455
4300	816.534	2158.254	1478.522	2922.846	326.882	2416.922	-29.359
4400	817.183	2177.033	1494.185	3004.533	322.700	2465.574	-29.269
4500	817.791	2195.405	1509.564	3086.282	318.253	2514.367	-29.185
4600	818.361	2213.385	1524.670	3168.090	313.499	2563.271	-29.106
4700	818.897	2230.991	1539.511	3249.953	308.451	2612.189	-29.031
4800	819.401	2248.237	1554.098	3331.868	303.144	2661.304	-28.960
4900	819.875	2265.137	1568.437	3413.832	297.520	2710.421	-28.893
5000	820.322	2281.705	1582.537	3495.842	291.654	2759.807	-28.831

3.118. Indeno[1,2,3-*cd*]fluoranthene



Formula: C₂₂H₁₂
Mass: 276.331 g/mol
CAS Number: 193-43-1
Point Group: D_{2h}

Length: 14.74 Å
Width: 9.102 Å
Breadth: 3.884 Å
L/B Ratio: 1.619

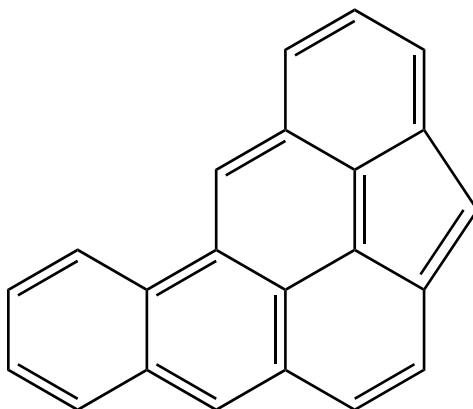
Cartesian coordinates:

C	4.0146	1.4164	0.0000	C	-1.4307	1.2075	0.0000	H	-4.0247	-2.5108	0.0000
C	2.8258	0.7215	0.0000	C	-0.7199	2.3839	0.0000	H	-4.0234	2.5128	0.0000
C	2.8255	-0.7229	0.0000	C	0.7211	2.3835	0.0000	H	1.2384	3.3485	0.0000
C	4.0139	-1.4183	0.0000	C	1.4313	1.2067	0.0000	H	-1.2368	3.3491	0.0000
C	5.2153	-0.6935	0.0000	C	-2.8255	0.7228	0.0000	H	-1.2385	-3.3484	0.0000
C	5.2156	0.6910	0.0000	C	-4.0139	1.4183	0.0000	H	1.2367	-3.3492	0.0000
C	1.4307	-1.2075	0.0000	C	-5.2153	0.6935	0.0000	H	4.0234	-2.5128	0.0000
C	0.6773	-0.0002	0.0000	C	-5.2156	-0.6910	0.0000	H	6.1656	-1.2377	0.0000
C	-0.6773	0.0003	0.0000	C	-4.0146	-1.4164	0.0000	H	6.1662	1.2346	0.0000
C	-1.4312	-1.2067	0.0000	C	-2.8258	-0.7215	0.0000	H	4.0247	2.5108	0.0000
C	-0.7211	-2.3835	0.0000	H	-6.1656	1.2376	0.0000				
C	0.7199	-2.3839	0.0000	H	-6.1662	-1.2346	0.0000				

Table 3.118: Table of thermodynamic data as a function of temperature for Indeno[1,2,3-*cd*]fluoranthene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-40.029	464.635	464.635	∞
100	87.943	308.872	653.140	-34.427	484.818	516.461	-269.766
200	171.748	393.922	502.317	-21.679	474.230	552.301	-144.243
250	221.661	437.559	484.978	-11.855	469.166	572.403	-119.595
298.15	270.665	480.798	480.798	0.000	464.635	592.709	-103.838
300	272.528	482.478	480.803	0.502	464.467	593.502	-103.336
350	321.558	528.207	484.303	15.367	460.276	615.349	-91.834
400	367.041	574.160	492.663	32.599	456.621	637.750	-83.280
450	408.226	619.813	504.260	51.999	453.440	660.586	-76.677
500	445.015	664.765	518.070	73.348	450.661	683.771	-71.432
600	506.636	751.573	549.817	121.054	446.077	730.846	-63.624
700	555.283	833.468	584.550	174.243	442.632	778.599	-58.099
800	594.223	910.251	620.516	231.788	440.197	826.764	-53.981
900	625.892	982.131	656.746	292.846	438.641	875.175	-50.793
1000	652.003	1049.469	692.688	356.782	437.846	923.727	-48.250
1100	673.766	1112.663	728.025	423.102	437.665	972.337	-46.171
1200	692.068	1172.095	762.579	491.420	437.992	1020.925	-44.439
1300	707.573	1228.119	796.256	561.423	438.691	1069.478	-42.971
1400	720.794	1281.053	829.011	632.858	439.663	1117.970	-41.711
1500	732.134	1331.179	860.833	705.519	440.848	1166.387	-40.616
1600	741.915	1378.750	891.729	779.233	442.146	1214.713	-39.655
1700	750.395	1423.988	921.719	853.858	443.503	1262.937	-38.805
1800	757.784	1467.094	950.829	929.276	444.863	1311.131	-38.047
1900	764.253	1508.242	979.092	1005.385	446.202	1359.208	-37.366
2000	769.941	1547.591	1006.541	1082.100	447.479	1407.238	-36.753
2100	774.964	1585.280	1033.209	1159.351	448.636	1455.194	-36.195
2200	779.418	1621.437	1059.130	1237.074	449.671	1503.100	-35.687
2300	783.383	1656.172	1084.338	1315.218	450.583	1550.962	-35.223
2400	786.925	1689.589	1108.865	1393.737	451.315	1598.749	-34.795
2500	790.101	1721.778	1132.742	1472.591	451.880	1646.599	-34.403
2600	792.958	1752.823	1155.998	1551.746	452.247	1694.337	-34.039
2700	795.537	1782.799	1178.661	1631.173	452.422	1742.123	-33.703
2800	797.870	1811.774	1200.757	1710.845	452.384	1789.923	-33.391
2900	799.989	1839.809	1222.313	1790.740	452.111	1837.686	-33.100
3000	801.917	1866.963	1243.351	1870.837	451.638	1885.484	-32.829
3100	803.677	1893.287	1263.894	1951.118	450.903	1933.238	-32.574
3200	805.287	1918.829	1283.964	2031.567	449.940	1981.080	-32.337
3300	806.764	1943.632	1303.580	2112.171	448.736	2028.988	-32.116
3400	808.121	1967.736	1322.761	2192.916	447.267	2076.865	-31.906
3500	809.370	1991.180	1341.525	2273.791	445.538	2124.775	-31.710
3600	810.524	2013.997	1359.890	2354.787	443.568	2172.809	-31.526
3700	811.591	2036.219	1377.870	2435.893	441.330	2220.914	-31.353
3800	812.579	2057.876	1395.481	2517.102	438.805	2269.036	-31.189
3900	813.496	2078.995	1412.737	2598.407	436.026	2317.185	-31.035
4000	814.349	2099.602	1429.652	2679.799	432.978	2365.521	-30.890
4100	815.143	2119.721	1446.239	2761.274	429.635	2413.877	-30.753
4200	815.884	2139.373	1462.509	2842.826	426.019	2462.311	-30.623
4300	816.576	2158.579	1478.474	2924.450	422.118	2510.762	-30.499
4400	817.223	2177.359	1494.145	3006.140	417.941	2559.381	-30.383
4500	817.829	2195.731	1509.533	3087.893	413.498	2608.142	-30.274
4600	818.398	2213.712	1524.646	3169.704	408.747	2657.013	-30.171
4700	818.932	2231.319	1539.495	3251.571	403.702	2705.899	-30.072
4800	819.434	2248.566	1554.089	3333.490	398.399	2754.980	-29.980
4900	819.907	2265.467	1568.435	3415.457	392.778	2804.065	-29.891
5000	820.353	2282.035	1582.541	3497.470	386.915	2853.418	-29.809

3.119. Phenanthro[10,1,2,3-*cdef*]fluorene



Formula: C₂₂H₁₂
Mass: 276.331 g/mol
CAS Number: 189-75-3
Point Group: C_s

Length: 13.78 Å
Width: 10.15 Å
Breadth: 3.885 Å
L/B Ratio: 1.357

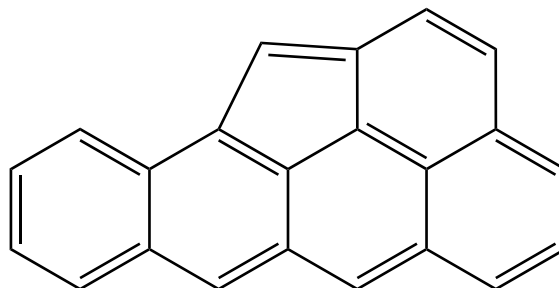
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C	1.5696	1.6331	0.0000	C	1.9959	-1.9994	0.0000	H	-4.9077	-1.2692	0.0000
C	2.0450	0.3249	0.0000	C	-2.1433	0.7463	0.0000	H	-2.1778	2.9003	0.0000
C	3.4012	-0.1434	0.0000	C	-2.9036	-0.4441	0.0000	H	-2.9320	-2.6360	0.0000
C	4.3578	0.8315	0.0000	C	-2.2834	-1.7519	0.0000	H	-0.7639	-4.0401	0.0000
C	3.9302	2.2003	0.0000	C	-4.3096	-0.3504	0.0000	H	1.6951	-4.1717	0.0000
C	0.1590	1.7835	0.0000	C	-4.9340	0.8803	0.0000	H	-0.2944	2.7865	0.0000
C	-0.6936	0.6717	0.0000	C	-4.1755	2.0578	0.0000	H	5.4279	0.6038	0.0000
C	-0.1622	-0.6477	0.0000	C	-2.7975	1.9904	0.0000	H	4.7176	2.9631	0.0000
C	1.1982	-0.7817	0.0000	C	3.3193	-1.6287	0.0000	H	2.3600	3.6717	0.0000
C	-0.9285	-1.8683	0.0000	H	4.1927	-2.2763	0.0000				
C	-0.1663	-3.1206	0.0000	H	-4.6803	3.0293	0.0000				

Table 3.119: Table of thermodynamic data as a function of temperature for Phenanthro[10,1,2,3-*cdef*]fluorene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-39.667	481.665	481.665	∞
100	84.330	317.292	659.860	-34.257	502.019	532.820	-278.311
200	171.285	400.818	509.367	-21.710	491.229	567.921	-148.323
250	222.070	444.457	491.995	-11.884	486.167	587.680	-122.786
298.15	271.423	487.803	487.803	0.000	481.665	607.651	-106.456
300	273.293	489.488	487.808	0.504	481.499	608.431	-105.935
350	322.399	535.343	491.318	15.409	477.348	629.924	-94.009
400	367.839	581.406	499.701	32.682	473.735	651.966	-85.136
450	408.944	627.148	511.325	52.120	470.592	674.437	-78.285
500	445.648	672.172	525.166	73.503	467.846	697.253	-72.840
600	507.121	759.081	556.974	121.264	463.318	743.582	-64.733
700	555.657	841.043	591.762	174.496	459.916	790.581	-58.993
800	594.515	917.869	627.777	232.074	457.514	837.986	-54.714
900	626.121	989.780	664.048	293.159	455.984	885.633	-51.400
1000	652.184	1057.140	700.025	357.114	455.210	933.420	-48.756
1100	673.911	1120.349	735.394	423.451	455.044	981.261	-46.595
1200	692.185	1179.793	769.975	491.782	455.385	1029.080	-44.794
1300	707.667	1235.825	803.675	561.795	456.095	1076.864	-43.268
1400	720.871	1288.765	836.451	633.239	457.075	1124.585	-41.958
1500	732.198	1338.896	868.291	705.907	458.266	1172.230	-40.820
1600	741.968	1386.471	899.204	779.627	459.570	1219.784	-39.821
1700	750.440	1431.712	929.208	854.257	460.933	1267.235	-38.937
1800	757.822	1474.820	958.332	929.679	462.296	1314.657	-38.150
1900	764.285	1515.970	986.607	1005.791	463.639	1361.962	-37.442
2000	769.968	1555.321	1014.066	1082.510	464.919	1409.218	-36.804
2100	774.988	1593.011	1040.743	1159.763	466.078	1456.402	-36.225
2200	779.439	1629.169	1066.674	1237.489	467.116	1503.534	-35.698
2300	783.401	1663.905	1091.890	1315.634	468.030	1550.623	-35.215
2400	786.941	1697.323	1116.425	1394.155	468.764	1597.636	-34.771
2500	790.115	1729.513	1140.308	1473.010	469.330	1644.713	-34.364
2600	792.971	1760.558	1163.571	1552.167	469.698	1691.677	-33.986
2700	795.548	1790.534	1186.240	1631.595	469.874	1738.690	-33.636
2800	797.881	1819.509	1208.342	1711.268	469.838	1785.717	-33.312
2900	799.998	1847.545	1229.903	1791.164	469.565	1832.706	-33.010
3000	801.926	1874.700	1250.946	1871.262	469.093	1879.730	-32.728
3100	803.685	1901.024	1271.494	1951.544	468.359	1926.711	-32.464
3200	805.294	1926.565	1291.567	2031.994	467.397	1973.780	-32.218
3300	806.770	1951.369	1311.187	2112.598	466.193	2020.914	-31.988
3400	808.126	1975.474	1330.372	2193.344	464.725	2068.017	-31.771
3500	809.376	1998.917	1349.140	2274.220	462.997	2115.153	-31.566
3600	810.529	2021.735	1367.508	2355.216	461.027	2162.414	-31.375
3700	811.595	2043.957	1385.491	2436.323	458.790	2209.745	-31.195
3800	812.583	2065.614	1403.106	2517.532	456.265	2257.093	-31.025
3900	813.500	2086.733	1420.365	2598.837	453.486	2304.468	-30.864
4000	814.353	2107.340	1437.283	2680.230	450.439	2352.030	-30.714
4100	815.146	2127.459	1453.872	2761.705	447.097	2399.613	-30.571
4200	815.887	2147.111	1470.145	2843.257	443.481	2447.273	-30.436
4300	816.579	2166.317	1486.112	2924.881	439.580	2494.950	-30.307
4400	817.226	2185.097	1501.786	3006.572	435.403	2542.795	-30.186
4500	817.832	2203.470	1517.175	3088.325	430.960	2590.782	-30.072
4600	818.400	2221.451	1532.291	3170.137	426.210	2638.880	-29.965
4700	818.934	2239.057	1547.142	3252.004	421.165	2686.991	-29.862
4800	819.436	2256.304	1561.737	3333.923	415.862	2735.299	-29.765
4900	819.909	2273.205	1576.085	3415.890	410.241	2783.610	-29.673
5000	820.355	2289.774	1590.193	3497.903	404.379	2832.189	-29.587

3.120. Indeno[6,7,1,2-*defg*]naphthacene



Formula: $C_{22}H_{12}$
Mass: 276.331 g/mol
CAS Number: 777080-15-6
Point Group: C_s

Length: 14.11 Å
Width: 9.550 Å
Breadth: 3.887 Å
L/B Ratio: 1.478

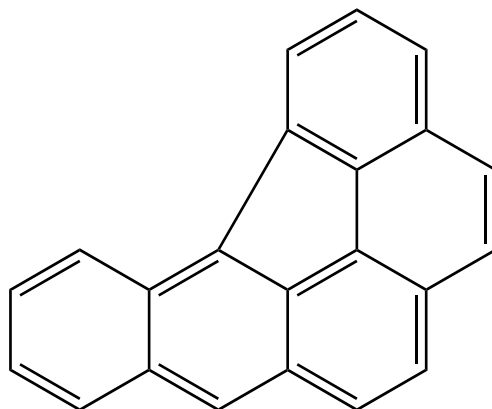
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C	-2.0290	1.5944	0.0000	C	-4.5306	0.1730	0.0000	H	-5.4089	2.1518	0.0000
C	-0.7666	2.2028	0.0000	C	-4.4606	1.6025	0.0000	H	-5.5136	-0.3099	0.0000
C	0.4284	1.4305	0.0000	C	-3.2837	2.2933	0.0000	H	-4.2213	-2.5711	0.0000
C	0.2669	0.0405	0.0000	C	0.5176	-2.2698	0.0000	H	-2.0882	-3.8052	0.0000
C	1.7834	1.8369	0.0000	H	1.0068	-3.2411	0.0000				
C	2.8047	0.8821	0.0000	H	5.8151	-1.6455	0.0000				

Table 3.120: Table of thermodynamic data as a function of temperature for Indeno[6,7,1,2-*defg*]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-39.751	511.315	511.315	∞
100	84.267	316.703	660.479	-34.378	531.547	562.407	-293.765
200	171.971	400.429	509.417	-21.798	520.791	597.560	-156.064
250	222.984	444.249	491.975	-11.931	515.769	617.334	-128.982
298.15	272.447	487.767	487.767	0.000	511.315	637.311	-111.652
300	274.320	489.458	487.772	0.506	511.150	638.091	-111.099
350	323.461	535.475	491.294	15.463	507.052	659.582	-98.435
400	368.892	581.679	499.705	32.790	503.492	681.613	-89.008
450	409.961	627.544	511.367	52.280	500.400	704.068	-81.724
500	446.616	672.672	525.248	73.712	497.705	726.861	-75.933
600	507.978	759.748	557.140	121.565	493.267	773.131	-67.306
700	556.405	841.833	592.009	174.877	489.946	820.057	-61.192
800	595.167	918.754	628.098	232.525	487.613	867.378	-56.633
900	626.691	990.736	664.436	293.670	486.144	914.933	-53.100
1000	652.685	1058.152	700.473	357.679	485.424	962.621	-50.281
1100	674.353	1121.407	735.895	424.063	485.306	1010.359	-47.977
1200	692.577	1180.887	770.524	492.435	485.688	1058.070	-46.056
1300	708.017	1236.949	804.268	562.486	486.434	1105.743	-44.428
1400	721.185	1289.913	837.082	633.963	487.448	1153.350	-43.031
1500	732.480	1340.065	868.958	706.660	488.669	1200.880	-41.817
1600	742.224	1387.656	899.902	780.407	490.000	1248.316	-40.752
1700	750.672	1432.913	929.935	855.062	491.387	1295.648	-39.810
1800	758.033	1476.033	959.086	930.505	492.772	1342.949	-38.971
1900	764.478	1517.195	987.385	1006.638	494.135	1390.132	-38.217
2000	770.145	1556.554	1014.867	1083.375	495.434	1437.265	-37.537
2100	775.150	1594.253	1041.565	1160.645	496.610	1484.325	-36.920
2200	779.589	1630.418	1067.515	1238.386	497.663	1531.333	-36.358
2300	783.540	1665.161	1092.749	1316.546	498.591	1578.297	-35.844
2400	787.070	1698.584	1117.300	1395.080	499.339	1625.184	-35.370
2500	790.235	1730.779	1141.200	1473.948	499.917	1672.135	-34.937
2600	793.082	1761.829	1164.476	1553.117	500.297	1718.972	-34.534
2700	795.652	1791.809	1187.159	1632.555	500.484	1765.858	-34.162
2800	797.978	1820.788	1209.274	1712.239	500.457	1812.756	-33.817
2900	800.089	1848.827	1230.847	1792.144	500.195	1859.618	-33.495
3000	802.011	1875.985	1251.901	1872.250	499.731	1906.513	-33.195
3100	803.765	1902.311	1272.460	1952.541	499.005	1953.366	-32.913
3200	805.370	1927.856	1292.544	2032.999	498.051	2000.305	-32.651
3300	806.842	1952.661	1312.173	2113.610	496.855	2047.310	-32.406
3400	808.194	1976.768	1331.367	2194.363	495.394	2094.284	-32.174
3500	809.440	2000.214	1350.144	2275.246	493.672	2141.291	-31.956
3600	810.590	2023.033	1368.519	2356.248	491.708	2188.422	-31.753
3700	811.653	2045.257	1386.511	2437.361	489.477	2235.623	-31.561
3800	812.638	2066.915	1404.132	2518.576	486.958	2282.841	-31.379
3900	813.552	2088.036	1421.399	2599.886	484.185	2330.086	-31.207
4000	814.402	2108.644	1438.323	2681.284	481.143	2377.518	-31.047
4100	815.194	2128.764	1454.919	2762.764	477.805	2424.970	-30.894
4200	815.932	2148.417	1471.198	2844.321	474.194	2472.499	-30.749
4300	816.622	2167.624	1487.171	2925.949	470.298	2520.046	-30.612
4400	817.267	2186.406	1502.850	3007.644	466.125	2567.760	-30.483
4500	817.871	2204.779	1518.245	3089.401	461.686	2615.616	-30.361
4600	818.438	2222.761	1533.366	3171.217	456.940	2663.583	-30.245
4700	818.971	2240.368	1548.222	3253.088	451.898	2711.563	-30.135
4800	819.471	2257.616	1562.822	3335.010	446.599	2759.740	-30.031
4900	819.943	2274.517	1577.174	3416.981	440.982	2807.919	-29.932
5000	820.387	2291.087	1591.288	3498.998	435.122	2856.367	-29.840

3.121. Naphtho[4,5,6-*abc*]aceanthrylene



Formula: C₂₂H₁₂
Mass: 276.331 g/mol
CAS Number: 777080-16-7
Point Group: C_s

Length: 13.30 Å
Width: 10.68 Å
Breadth: 3.885 Å
L/B Ratio: 1.246

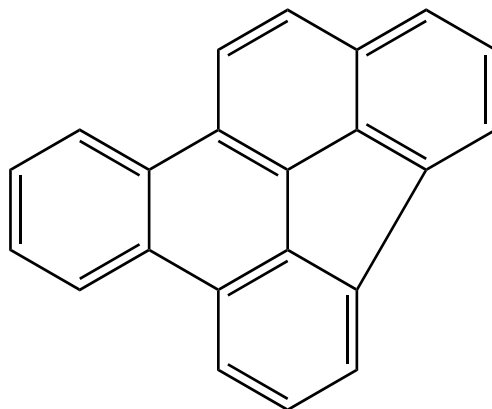
Cartesian coordinates:

C	-1.7779	-0.3678	0.0000	C	0.9812	1.9414	0.0000	H	4.8961	0.9444	0.0000
C	-0.7221	-1.3425	0.0000	C	0.2561	3.1990	0.0000	H	1.7905	-2.9698	0.0000
C	0.5482	-0.5604	0.0000	C	-1.1121	3.2825	0.0000	H	3.0783	2.4925	0.0000
C	0.1773	0.8019	0.0000	C	-1.9487	2.1018	0.0000	H	0.8551	4.1167	0.0000
C	-1.2362	0.9328	0.0000	C	-3.3717	1.9070	0.0000	H	-1.6039	4.2611	0.0000
C	3.8296	-2.3029	0.0000	C	-3.9315	0.6462	0.0000	H	-4.0180	2.7912	0.0000
C	4.7084	-1.1845	0.0000	C	-3.1464	-0.5606	0.0000	H	-5.0222	0.5403	0.0000
C	4.2159	0.0844	0.0000	C	-3.5239	-1.9322	0.0000	H	-4.5845	-2.2031	0.0000
C	2.4810	-2.1181	0.0000	C	-2.5461	-2.9062	0.0000	H	-2.8557	-3.9578	0.0000
C	1.9261	-0.8021	0.0000	C	-1.1422	-2.6464	0.0000	H	-0.4393	-3.4858	0.0000
C	2.8045	0.3342	0.0000	H	4.2577	-3.3106	0.0000				
C	2.3509	1.6727	0.0000	H	5.7885	-1.3646	0.0000				

Table 3.121: Table of thermodynamic data as a function of temperature for Naphtho[4,5,6-*abc*]aceanthrylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-39.584	452.969	452.969	∞
100	84.589	318.035	659.315	-34.128	473.451	504.178	-263.350
200	170.535	401.384	509.446	-21.612	462.631	539.209	-140.824
250	221.050	444.824	492.151	-11.832	457.523	558.944	-116.783
298.15	270.275	487.978	487.978	0.000	452.969	578.902	-101.419
300	272.142	489.656	487.983	0.502	452.801	579.682	-100.930
350	321.221	535.331	491.478	15.348	448.591	601.172	-89.718
400	366.697	581.238	499.830	32.563	444.920	623.218	-81.382
450	407.871	626.849	511.414	51.946	441.721	645.701	-74.949
500	444.659	671.764	525.210	73.277	438.924	668.535	-69.840
600	506.309	758.509	556.928	120.948	434.306	714.913	-62.237
700	555.005	840.357	591.632	174.107	430.831	761.976	-56.858
800	593.996	917.106	627.572	231.627	428.370	809.453	-52.851
900	625.711	988.962	663.779	292.665	426.794	857.180	-49.748
1000	651.858	1056.283	699.699	356.584	425.983	905.050	-47.274
1100	673.652	1119.465	735.018	422.892	425.789	952.979	-45.252
1200	691.977	1178.888	769.556	491.199	426.106	1000.887	-43.567
1300	707.500	1234.906	803.218	561.194	426.797	1048.762	-42.139
1400	720.735	1287.834	835.961	632.623	427.762	1096.575	-40.913
1500	732.086	1337.957	867.771	705.278	428.941	1144.314	-39.848
1600	741.876	1385.525	898.657	778.988	430.235	1191.962	-38.913
1700	750.363	1430.761	928.638	853.610	431.589	1239.509	-38.085
1800	757.758	1473.865	957.740	929.025	432.946	1287.026	-37.348
1900	764.231	1515.012	985.996	1005.131	434.282	1334.426	-36.685
2000	769.922	1554.360	1013.438	1081.845	435.558	1381.778	-36.088
2100	774.948	1592.049	1040.099	1159.093	436.712	1429.058	-35.545
2200	779.404	1628.204	1066.015	1236.815	437.746	1476.287	-35.051
2300	783.371	1662.939	1091.218	1314.958	438.657	1523.472	-34.598
2400	786.915	1696.355	1115.741	1393.475	439.389	1570.582	-34.182
2500	790.093	1728.544	1139.613	1472.329	439.952	1617.756	-33.800
2600	792.951	1759.589	1162.865	1551.483	440.318	1664.817	-33.446
2700	795.530	1789.564	1185.524	1630.909	440.493	1711.927	-33.119
2800	797.865	1818.539	1207.617	1710.581	440.454	1759.050	-32.815
2900	799.984	1846.575	1229.169	1790.475	440.180	1806.137	-32.531
3000	801.913	1873.728	1250.204	1870.572	439.707	1853.258	-32.267
3100	803.673	1900.052	1270.745	1950.852	438.971	1900.336	-32.020
3200	805.284	1925.593	1290.812	2031.301	438.008	1947.502	-31.789
3300	806.761	1950.396	1310.425	2111.905	436.804	1994.733	-31.573
3400	808.118	1974.501	1329.604	2192.649	435.335	2041.934	-31.370
3500	809.368	1997.945	1348.366	2273.525	433.606	2089.167	-31.178
3600	810.522	2020.762	1366.728	2354.520	431.635	2136.525	-31.000
3700	811.589	2042.984	1384.706	2435.626	429.397	2183.953	-30.831
3800	812.577	2064.641	1402.316	2516.835	426.872	2231.398	-30.672
3900	813.495	2085.760	1419.570	2598.139	424.092	2278.871	-30.521
4000	814.347	2106.367	1436.484	2679.532	421.045	2326.531	-30.381
4100	815.142	2126.485	1453.069	2761.007	417.702	2374.210	-30.247
4200	815.882	2146.137	1469.337	2842.558	414.086	2421.968	-30.121
4300	816.574	2165.343	1485.301	2924.182	410.185	2469.743	-30.001
4400	817.222	2184.123	1500.971	3005.872	406.007	2517.685	-29.888
4500	817.828	2202.495	1516.357	3087.625	401.564	2565.770	-29.782
4600	818.397	2220.477	1531.469	3169.436	396.813	2613.965	-29.682
4700	818.931	2238.083	1546.316	3251.303	391.768	2662.173	-29.586
4800	819.433	2255.330	1560.909	3333.221	386.464	2710.578	-29.496
4900	819.906	2272.231	1575.253	3415.188	380.844	2758.987	-29.411
5000	820.352	2288.800	1589.359	3497.202	374.981	2807.663	-29.331

3.122. Indeno[3,2,1,7-*defg*]chrysene



Other names: Dibenzo[*b,mno*]fluoranthene
Naphtho[1,2,3,4-*ghi*]fluoranthene

Formula: C₂₂H₁₂
Mass: 276.331 g/mol
CAS Number: 668-30-4
Point Group: C_s

Length: 13.34 Å
Width: 10.50 Å
Breadth: 3.885 Å
L/B Ratio: 1.271

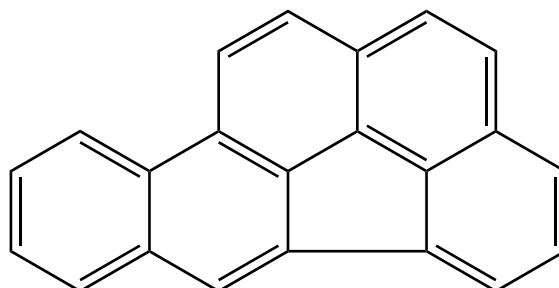
Cartesian coordinates:

C	2.2237	1.2024	0.0000	C	-0.2491	-1.4914	0.0000	H	3.9816	2.4570	0.0000
C	4.0518	-0.9943	0.0000	C	0.4443	-0.3136	0.0000	H	1.2513	4.1112	0.0000
C	4.4577	0.3235	0.0000	C	-0.1024	0.9994	0.0000	H	-1.1683	4.5991	0.0000
C	3.5705	1.4432	0.0000	C	-1.4653	1.2044	0.0000	H	-2.8983	2.8446	0.0000
C	0.9464	1.9696	0.0000	C	-1.6987	-1.3171	0.0000	H	0.1168	-3.6431	0.0000
C	0.5374	3.2824	0.0000	C	-2.2804	-0.0113	0.0000	H	2.5720	-3.4740	0.0000
C	-0.8558	3.5486	0.0000	C	-3.6800	0.1027	0.0000	H	-4.1295	1.1042	0.0000
C	-1.8371	2.5692	0.0000	C	-4.4876	-1.0185	0.0000	H	-5.5772	-0.9104	0.0000
C	2.6620	-1.3017	0.0000	C	-3.9172	-2.2939	0.0000	H	-4.5627	-3.1783	0.0000
C	1.8477	-0.1839	0.0000	C	-2.5429	-2.4384	0.0000	H	-2.0971	-3.4406	0.0000
C	0.5911	-2.6547	0.0000	H	4.7856	-1.8068	0.0000				
C	1.9680	-2.5597	0.0000	H	5.5320	0.5412	0.0000				

Table 3.122: Table of thermodynamic data as a function of temperature for Indeno[3,2,1,7-*defg*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-39.489	423.903	423.903	∞
100	84.950	316.972	657.551	-34.058	444.455	475.289	-248.260
200	170.121	400.445	508.092	-21.529	433.648	510.414	-133.304
250	220.159	443.737	490.867	-11.782	428.507	530.200	-110.777
298.15	269.142	486.711	486.711	0.000	423.903	550.214	-96.393
300	271.004	488.382	486.716	0.500	423.733	550.997	-95.935
350	319.999	533.873	490.197	15.287	419.464	572.554	-85.447
400	365.483	579.617	498.516	32.440	415.732	594.678	-77.655
450	406.710	625.088	510.058	51.764	412.473	617.245	-71.646
500	443.569	669.885	523.808	73.038	409.620	640.170	-66.877
600	505.367	756.444	555.430	120.608	404.900	686.746	-59.785
700	554.193	838.157	590.043	173.680	401.337	734.023	-54.772
800	593.290	914.805	625.900	231.124	398.801	781.725	-51.040
900	625.090	986.582	662.032	292.095	397.159	829.686	-48.153
1000	651.309	1053.842	697.886	355.956	396.290	877.797	-45.850
1100	673.162	1116.974	733.145	422.212	396.043	925.973	-43.970
1200	691.537	1176.357	767.630	490.473	396.314	974.132	-42.402
1300	707.104	1232.341	801.244	560.426	396.963	1022.262	-41.074
1400	720.376	1285.242	833.944	631.817	397.891	1070.333	-39.934
1500	731.761	1335.341	865.715	704.438	399.036	1118.333	-38.943
1600	741.580	1382.889	896.565	778.117	400.299	1166.243	-38.073
1700	750.093	1428.108	926.513	852.711	401.624	1214.054	-37.303
1800	757.510	1471.197	955.586	928.099	402.955	1261.837	-36.617
1900	764.002	1512.331	983.814	1004.182	404.267	1309.505	-36.000
2000	769.712	1551.668	1011.231	1080.874	405.521	1357.126	-35.444
2100	774.754	1589.346	1037.869	1158.102	406.655	1404.675	-34.939
2200	779.225	1625.493	1063.763	1235.806	407.671	1452.175	-34.478
2300	783.204	1660.221	1088.946	1313.931	408.564	1499.632	-34.057
2400	786.760	1693.630	1113.450	1392.432	409.280	1547.014	-33.669
2500	789.948	1725.813	1137.305	1471.271	409.828	1594.461	-33.314
2600	792.816	1756.852	1160.540	1550.411	410.180	1641.795	-32.983
2700	795.404	1786.823	1183.184	1629.824	410.342	1689.179	-32.678
2800	797.746	1815.793	1205.263	1709.484	410.291	1736.577	-32.396
2900	799.873	1843.824	1226.801	1789.366	410.006	1783.938	-32.132
3000	801.808	1870.974	1247.824	1869.452	409.521	1831.334	-31.886
3100	803.575	1897.295	1268.352	1949.722	408.776	1878.688	-31.655
3200	805.191	1922.833	1288.407	2030.162	407.803	1926.130	-31.440
3300	806.672	1947.633	1308.010	2110.756	406.589	1973.637	-31.239
3400	808.034	1971.735	1327.179	2191.492	405.112	2021.114	-31.050
3500	809.289	1995.176	1345.931	2272.359	403.375	2068.624	-30.872
3600	810.447	2017.991	1364.284	2353.347	401.396	2116.259	-30.705
3700	811.517	2040.211	1382.253	2434.446	399.151	2163.964	-30.549
3800	812.509	2061.866	1399.854	2515.648	396.619	2211.687	-30.401
3900	813.430	2082.984	1417.100	2596.945	393.832	2259.437	-30.261
4000	814.286	2103.589	1434.006	2678.331	390.779	2307.375	-30.131
4100	815.083	2123.706	1450.584	2759.800	387.430	2355.332	-30.007
4200	815.826	2143.356	1466.845	2841.346	383.807	2403.368	-29.890
4300	816.521	2162.561	1482.802	2922.964	379.901	2451.421	-29.778
4400	817.170	2181.340	1498.466	3004.649	375.718	2499.641	-29.674
4500	817.779	2199.711	1513.845	3086.397	371.270	2548.004	-29.576
4600	818.349	2217.691	1528.952	3168.203	366.515	2596.477	-29.483
4700	818.886	2235.297	1543.794	3250.065	361.465	2644.965	-29.395
4800	819.390	2252.543	1558.380	3331.979	356.157	2693.648	-29.312
4900	819.864	2269.443	1572.720	3413.942	350.532	2742.336	-29.233
5000	820.312	2286.011	1586.820	3495.951	344.665	2791.291	-29.160

3.123. Indeno[4,3,2,1-*cdef*]chrysene



Other names: Dibenzo[*b,ghi*]fluoranthene
Indeno[7,1,2,3-*cdef*]chrysene

Formula: C₂₂H₁₂
Mass: 276.331 g/mol
CAS Number: 203-25-8
Point Group: C_s

Length: 13.77 Å
Width: 9.862 Å
Breadth: 3.885 Å
L/B Ratio: 1.396

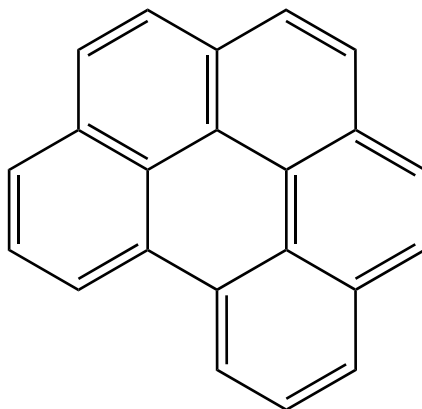
Cartesian coordinates:

C	0.0273	1.2052	0.0000	C	-1.3464	-2.1981	0.0000	H	5.9327	-0.5676	0.0000
C	1.1833	1.9123	0.0000	C	-1.0950	-0.8463	0.0000	H	5.7875	1.9103	0.0000
C	2.4434	1.1892	0.0000	C	-3.7199	-1.5432	0.0000	H	3.5822	3.0346	0.0000
C	2.5351	-0.2289	0.0000	C	-2.7520	-2.5197	0.0000	H	-0.2600	-4.0876	0.0000
C	3.8017	-0.8441	0.0000	C	-3.4158	-0.1311	0.0000	H	1.9836	-3.0735	0.0000
C	4.9503	-0.0842	0.0000	C	-2.0696	0.1779	0.0000	H	-4.7777	-1.8291	0.0000
C	4.8677	1.3163	0.0000	C	-1.4404	1.4647	0.0000	H	-3.0398	-3.5764	0.0000
C	3.6398	1.9396	0.0000	C	-2.2988	2.5337	0.0000	H	-1.9409	3.5674	0.0000
C	1.3151	-1.0052	0.0000	C	-3.6998	2.2728	0.0000	H	-4.3683	3.1415	0.0000
C	0.1738	-0.2388	0.0000	C	-4.2608	1.0098	0.0000	H	-5.3478	0.8810	0.0000
C	-0.1584	-2.9972	0.0000	H	1.2036	3.0073	0.0000				
C	1.0997	-2.4239	0.0000	H	3.8595	-1.9394	0.0000				

Table 3.123: Table of thermodynamic data as a function of temperature for Indeno[4,3,2,1-*cdef*]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-39.434	427.573	427.573	∞
100	84.280	317.176	657.404	-34.023	448.161	478.974	-250.185
200	169.955	400.243	507.991	-21.550	437.298	514.104	-134.268
250	220.399	443.544	490.745	-11.800	432.159	533.900	-111.550
298.15	269.620	486.583	486.583	0.000	427.573	553.923	-97.043
300	271.488	488.257	486.588	0.501	427.404	554.705	-96.581
350	320.598	533.833	490.075	15.315	423.163	576.267	-86.001
400	366.118	579.660	498.410	32.500	419.461	598.390	-78.140
450	407.337	625.205	509.972	51.855	416.234	620.954	-72.077
500	444.169	670.067	523.746	73.160	413.412	643.872	-67.263
600	505.897	756.729	555.417	120.787	408.748	690.424	-60.105
700	554.659	838.519	590.079	173.908	405.235	737.668	-55.044
800	593.704	915.225	625.981	231.396	402.743	785.331	-51.276
900	625.462	987.049	662.153	292.407	401.140	833.247	-48.359
1000	651.646	1054.346	698.043	356.303	400.306	881.310	-46.034
1100	673.469	1117.509	733.335	422.591	400.092	929.433	-44.134
1200	691.818	1176.918	767.850	490.881	400.392	977.538	-42.550
1300	707.361	1232.923	801.492	560.861	401.068	1025.610	-41.209
1400	720.613	1285.842	834.216	632.277	402.020	1073.623	-40.057
1500	731.978	1335.956	866.009	704.921	403.188	1121.562	-39.055
1600	741.780	1383.518	896.880	778.621	404.472	1169.410	-38.177
1700	750.277	1428.749	926.847	853.233	405.817	1217.157	-37.398
1800	757.680	1471.848	955.937	928.640	407.165	1264.876	-36.705
1900	764.161	1512.991	984.181	1004.739	408.494	1312.478	-36.082
2000	769.858	1552.335	1011.612	1081.446	409.763	1360.032	-35.520
2100	774.890	1590.021	1038.265	1158.688	410.912	1407.515	-35.009
2200	779.351	1626.174	1064.172	1236.405	411.940	1454.947	-34.544
2300	783.323	1660.907	1089.367	1314.542	412.846	1502.335	-34.118
2400	786.870	1694.321	1113.881	1393.055	413.573	1549.648	-33.727
2500	790.051	1726.508	1137.747	1471.904	414.132	1597.026	-33.367
2600	792.912	1757.551	1160.992	1551.055	414.494	1644.290	-33.034
2700	795.494	1787.525	1183.645	1630.477	414.665	1691.604	-32.725
2800	797.832	1816.499	1205.732	1710.145	414.623	1738.931	-32.439
2900	799.953	1844.533	1227.279	1790.036	414.346	1786.222	-32.173
3000	801.884	1871.686	1248.309	1870.130	413.869	1833.547	-31.924
3100	803.646	1898.009	1268.845	1950.408	413.131	1880.830	-31.691
3200	805.258	1923.549	1288.907	2030.854	412.165	1928.200	-31.474
3300	806.737	1948.351	1308.517	2111.455	410.958	1975.635	-31.271
3400	808.095	1972.455	1327.691	2192.197	409.487	2023.041	-31.080
3500	809.347	1995.898	1346.450	2273.070	407.756	2070.479	-30.900
3600	810.502	2018.715	1364.808	2354.063	405.783	2118.041	-30.731
3700	811.569	2040.936	1382.783	2435.168	403.543	2165.674	-30.573
3800	812.559	2062.593	1400.389	2516.375	401.016	2213.324	-30.424
3900	813.477	2083.711	1417.640	2597.677	398.234	2261.002	-30.282
4000	814.331	2104.318	1434.551	2679.068	395.185	2308.866	-30.150
4100	815.126	2124.436	1451.133	2760.541	391.841	2356.751	-30.025
4200	815.867	2144.087	1467.399	2842.091	388.223	2404.713	-29.906
4300	816.560	2163.293	1483.360	2923.713	384.321	2452.693	-29.794
4400	817.208	2182.073	1499.027	3005.402	380.141	2500.840	-29.688
4500	817.815	2200.445	1514.411	3087.153	375.697	2549.130	-29.589
4600	818.384	2218.426	1529.521	3168.964	370.945	2597.530	-29.495
4700	818.919	2236.032	1544.366	3250.829	365.899	2645.944	-29.406
4800	819.422	2253.278	1558.956	3332.746	360.594	2694.554	-29.322
4900	819.895	2270.179	1573.299	3414.712	354.972	2743.168	-29.242
5000	820.341	2286.748	1587.403	3496.724	349.108	2792.049	-29.168

3.124. Benzo[ghi]perylene



Other names: 1,12-Benzoperylene

Formula: $C_{22}H_{12}$

Mass: 276.331 g/mol

CAS Number: 191-24-2

Point Group: C_{2v}

Length: 11.67 Å

Width: 10.40 Å

Breadth: 3.885 Å

L/B Ratio: 1.122

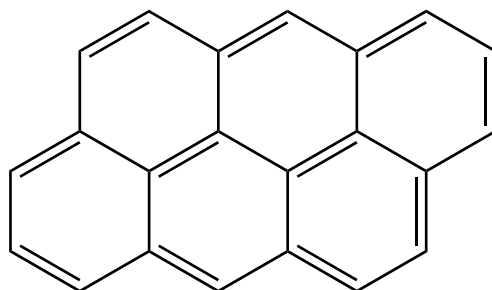
Cartesian coordinates:

C	0.7422	1.5737	0.0000	C	-1.4256	-2.1028	0.0000	H	0.9402	3.7142	0.0000
C	3.5518	1.5211	0.0000	C	-0.7185	-0.8934	0.0000	H	3.3463	-3.0871	0.0000
C	2.8749	2.7237	0.0000	C	-3.5329	-0.8991	0.0000	H	4.6141	-0.9525	0.0000
C	1.4766	2.7526	0.0000	C	-2.8592	-2.0770	0.0000	H	-1.2755	-4.2678	0.0000
C	2.8374	0.3080	0.0000	C	-2.8320	0.3536	0.0000	H	1.2067	-4.2878	0.0000
C	1.4285	0.3325	0.0000	C	-1.4229	0.3555	0.0000	H	-4.6288	-0.8781	0.0000
C	2.8253	-2.1228	0.0000	C	-0.7167	1.5855	0.0000	H	-3.3955	-3.0328	0.0000
C	3.5180	-0.9558	0.0000	C	-1.4321	2.7761	0.0000	H	-0.8803	3.7288	0.0000
C	1.3915	-2.1255	0.0000	C	-2.8307	2.7696	0.0000	H	-3.3716	3.7218	0.0000
C	0.7040	-0.9049	0.0000	C	-3.5268	1.5781	0.0000	H	-4.6227	1.5746	0.0000
C	-0.7120	-3.3277	0.0000	H	4.6474	1.4999	0.0000				
C	0.6583	-3.3388	0.0000	H	3.4309	3.6671	0.0000				

Table 3.124: Table of thermodynamic data as a function of temperature for Benzo[ghi]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-38.667	311.112	311.112	∞
100	80.213	305.868	641.075	-33.521	332.201	364.145	-190.206
200	167.762	386.782	493.515	-21.347	321.040	400.538	-104.608
250	218.361	429.618	476.423	-11.701	315.797	421.019	-87.965
298.15	267.543	472.295	472.295	0.000	311.112	441.721	-77.386
300	269.409	473.955	472.300	0.497	310.939	442.530	-77.050
350	318.486	519.208	475.762	15.206	306.592	464.816	-69.368
400	364.037	564.754	484.039	32.286	302.786	487.677	-63.683
450	405.345	610.059	495.529	51.539	299.457	510.992	-59.313
500	442.301	654.717	509.221	72.748	296.538	534.673	-55.856
600	504.308	741.063	540.728	120.201	291.702	582.776	-50.734
700	553.326	822.628	575.233	173.177	288.043	631.599	-47.129
800	592.582	899.171	610.993	230.542	285.428	680.860	-44.455
900	624.509	970.873	647.039	291.450	283.722	730.388	-42.390
1000	650.828	1038.077	682.819	355.258	282.800	780.073	-40.746
1100	672.759	1101.167	718.012	421.469	282.510	829.827	-39.404
1200	691.197	1160.517	752.440	489.693	282.743	879.569	-38.286
1300	706.812	1216.476	786.003	559.615	283.361	929.284	-37.338
1400	720.125	1269.357	818.657	630.979	284.261	978.943	-36.524
1500	731.542	1319.439	850.388	703.577	285.383	1028.532	-35.816
1600	741.388	1366.974	881.202	777.235	286.625	1078.033	-35.193
1700	749.923	1412.183	911.117	851.811	287.933	1127.436	-34.641
1800	757.359	1455.262	940.160	927.183	289.247	1176.813	-34.150
1900	763.867	1496.389	968.362	1003.252	290.546	1226.074	-33.706
2000	769.590	1535.719	995.753	1079.931	291.787	1275.289	-33.306
2100	774.644	1573.392	1022.369	1157.147	292.910	1324.434	-32.943
2200	779.125	1609.534	1048.243	1234.840	293.914	1373.530	-32.611
2300	783.113	1644.257	1073.407	1312.956	294.798	1422.583	-32.307
2400	786.676	1677.663	1097.892	1391.449	295.505	1471.561	-32.027
2500	789.871	1709.842	1121.731	1470.279	296.045	1520.605	-31.771
2600	792.745	1740.878	1144.951	1549.412	296.390	1569.536	-31.532
2700	795.338	1770.846	1167.580	1628.818	296.545	1618.518	-31.311
2800	797.685	1799.814	1189.646	1708.472	296.488	1667.513	-31.107
2900	799.816	1827.844	1211.172	1788.348	296.196	1716.472	-30.916
3000	801.755	1854.992	1232.182	1868.428	295.706	1765.467	-30.739
3100	803.525	1881.311	1252.700	1948.694	294.956	1814.419	-30.572
3200	805.144	1906.847	1272.745	2029.128	293.978	1863.459	-30.417
3300	806.629	1931.646	1292.338	2109.718	292.760	1912.565	-30.273
3400	807.993	1955.747	1311.497	2190.450	291.278	1961.641	-30.136
3500	809.250	1979.187	1330.240	2271.313	289.537	2010.750	-30.008
3600	810.410	2002.001	1348.585	2352.297	287.555	2059.984	-29.889
3700	811.483	2024.220	1366.546	2433.392	285.306	2109.288	-29.777
3800	812.476	2045.874	1384.140	2514.591	282.771	2158.610	-29.672
3900	813.399	2066.991	1401.379	2595.885	279.981	2207.959	-29.572
4000	814.256	2087.595	1418.278	2677.268	276.925	2257.496	-29.479
4100	815.055	2107.711	1434.849	2758.734	273.573	2307.053	-29.392
4200	815.799	2127.361	1451.104	2840.278	269.948	2356.688	-29.309
4300	816.495	2146.565	1467.055	2921.893	266.039	2406.341	-29.231
4400	817.146	2165.344	1482.713	3003.575	261.853	2456.161	-29.158
4500	817.755	2183.714	1498.087	3085.320	257.403	2506.123	-29.090
4600	818.327	2201.694	1513.189	3167.125	252.645	2556.196	-29.026
4700	818.864	2219.299	1528.026	3248.985	247.593	2606.284	-28.965
4800	819.369	2236.544	1542.607	3330.897	242.283	2656.567	-28.909
4900	819.845	2253.444	1556.942	3412.858	236.656	2706.854	-28.855
5000	820.293	2270.011	1571.039	3494.865	230.787	2757.409	-28.806

3.125. Dibenzo[*def,mno*]chrysene



Other names: Anthanthrene
Dibenzo[*cd,jk*]pyrene

Formula: C₂₂H₁₂

Mass: 276.331 g/mol

CAS Number: 191-26-4

Point Group: C_{2h}

Length: 12.84 Å

Width: 9.538 Å

Breadth: 3.885 Å

L/B Ratio: 1.346

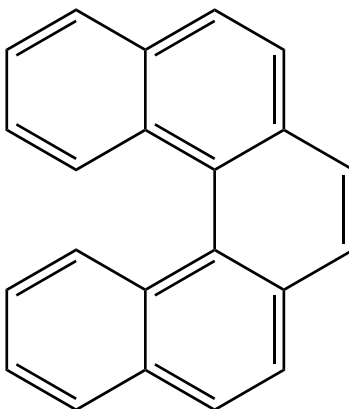
Cartesian coordinates:

C	4.2438	-0.5407	0.0000	C	-1.8724	0.0322	0.0000	H	3.7430	2.8364	0.0000
C	4.5279	0.8330	0.0000	C	-2.1632	-1.3499	0.0000	H	1.3366	3.3623	0.0000
C	3.5135	1.7648	0.0000	C	-1.0953	-2.2923	0.0000	H	-1.0732	3.8799	0.0000
C	2.1632	1.3499	0.0000	C	-0.5173	0.4707	0.0000	H	-3.4269	3.1078	0.0000
C	1.0953	2.2923	0.0000	C	0.5173	-0.4708	0.0000	H	-5.0666	1.2645	0.0000
C	-0.2129	1.8724	0.0000	C	0.2129	-1.8724	0.0000	H	-5.5729	-1.1610	0.0000
C	-1.3166	2.8110	0.0000	C	1.3165	-2.8111	0.0000	H	-3.7430	-2.8364	0.0000
C	-2.5976	2.3910	0.0000	C	2.5976	-2.3911	0.0000	H	-1.3365	-3.3624	0.0000
C	-2.9301	0.9820	0.0000	C	2.9302	-0.9820	0.0000	H	1.0731	-3.8799	0.0000
C	-4.2437	0.5408	0.0000	C	1.8725	-0.0323	0.0000	H	3.4269	-3.1079	0.0000
C	-4.5279	-0.8329	0.0000	H	5.0665	-1.2645	0.0000				
C	-3.5136	-1.7648	0.0000	H	5.5728	1.1613	0.0000				

Table 3.125: Table of thermodynamic data as a function of temperature for Dibenzo[def,mno]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-38.638	332.930	332.930	∞
100	79.645	304.669	640.251	-33.558	353.982	386.045	-201.645
200	168.046	385.462	492.445	-21.397	342.807	422.570	-110.362
250	218.901	428.392	475.312	-11.730	337.586	443.115	-92.582
298.15	268.167	471.174	471.174	0.000	332.930	463.873	-81.267
300	270.033	472.838	471.179	0.498	332.758	464.684	-80.907
350	319.083	518.186	474.648	15.238	328.442	487.023	-72.683
400	364.558	563.807	482.942	32.346	324.664	509.934	-66.589
450	405.779	609.169	494.451	51.623	321.359	533.295	-61.902
500	442.656	653.868	508.165	72.851	318.459	557.018	-58.190
600	504.548	740.268	539.711	120.334	313.652	605.204	-52.687
700	553.504	821.864	574.250	173.330	310.014	654.104	-48.809
800	592.730	898.428	610.039	230.712	307.415	703.441	-45.929
900	624.644	970.147	646.110	291.633	305.723	753.042	-43.705
1000	650.956	1037.365	681.910	355.454	304.814	802.799	-41.933
1100	672.884	1100.467	717.122	421.679	304.537	852.624	-40.487
1200	691.319	1159.828	751.566	489.915	304.783	902.435	-39.281
1300	706.931	1215.797	785.144	559.849	305.412	952.219	-38.260
1400	720.240	1268.686	817.811	631.225	306.324	1001.945	-37.382
1500	731.652	1318.776	849.554	703.833	307.457	1051.601	-36.619
1600	741.493	1366.318	880.379	777.503	308.710	1101.168	-35.949
1700	750.023	1411.533	910.304	852.088	310.028	1150.636	-35.354
1800	757.453	1454.618	939.357	927.471	311.352	1200.077	-34.825
1900	763.957	1495.749	967.566	1003.548	312.660	1249.403	-34.348
2000	769.675	1535.084	994.966	1080.236	313.910	1298.682	-33.917
2100	774.724	1572.761	1021.589	1157.461	315.041	1347.890	-33.526
2200	779.200	1608.907	1047.469	1235.162	316.053	1397.049	-33.169
2300	783.184	1643.633	1072.640	1313.285	316.944	1446.164	-32.843
2400	786.743	1677.042	1097.131	1391.784	317.658	1495.205	-32.542
2500	789.934	1709.224	1120.975	1470.621	318.205	1544.310	-32.266
2600	792.805	1740.263	1144.201	1549.760	318.556	1593.304	-32.009
2700	795.395	1770.233	1166.835	1629.173	318.716	1642.346	-31.772
2800	797.739	1799.202	1188.905	1708.831	318.665	1691.403	-31.553
2900	799.867	1827.234	1210.436	1788.713	318.379	1740.424	-31.348
3000	801.803	1854.384	1231.451	1868.798	317.894	1789.479	-31.157
3100	803.571	1880.704	1251.972	1949.068	317.148	1838.492	-30.978
3200	805.188	1906.242	1272.021	2029.507	316.175	1887.592	-30.811
3300	806.670	1931.042	1291.617	2110.101	314.961	1936.759	-30.656
3400	808.033	1955.144	1310.780	2190.837	313.483	1985.895	-30.509
3500	809.288	1978.585	1329.527	2271.704	311.746	2035.064	-30.371
3600	810.446	2001.400	1347.875	2352.692	309.767	2084.358	-30.243
3700	811.517	2023.620	1365.839	2433.790	307.522	2133.723	-30.122
3800	812.509	2045.275	1383.435	2514.992	304.990	2183.105	-30.008
3900	813.430	2066.393	1400.677	2596.290	302.204	2232.514	-29.901
4000	814.286	2086.998	1417.579	2677.676	299.150	2282.110	-29.801
4100	815.083	2107.115	1434.152	2759.145	295.801	2331.727	-29.706
4200	815.827	2126.765	1450.410	2840.691	292.179	2381.422	-29.617
4300	816.521	2145.970	1466.364	2922.309	288.273	2431.133	-29.532
4400	817.171	2164.749	1482.023	3003.994	284.090	2481.013	-29.453
4500	817.780	2183.120	1497.400	3085.742	279.641	2531.035	-29.379
4600	818.350	2201.100	1512.503	3167.548	274.886	2581.168	-29.309
4700	818.887	2218.706	1527.342	3249.411	269.836	2631.314	-29.243
4800	819.391	2235.952	1541.926	3331.325	264.529	2681.657	-29.182
4900	819.865	2252.852	1556.262	3413.288	258.904	2732.003	-29.123
5000	820.313	2269.420	1570.360	3495.297	253.037	2782.618	-29.069

3.126. Dibenzo[*c,g*]phenanthrene



Other names: 3,4,5,6-Dibenzophenanthrene
 γ,γ' -Dibenzophenanthrene
Formula: $C_{22}H_{14}$
Mass: 278.347 g/mol
CAS Number: 188-52-3
Point Group: C_2

Length: 11.94 Å
Width: 10.07 Å
Breadth: 5.996 Å
L/B Ratio: 1.186

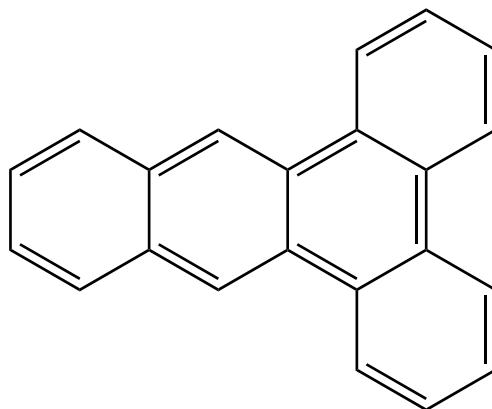
Cartesian coordinates:

C	-3.2773	-2.5837	-0.5506	C	1.3239	2.0071	-0.3887	H	0.1548	-1.5093	1.3090
C	-1.9742	-2.5853	-1.0788	C	0.7086	0.7845	-0.0796	H	-4.7662	-1.4486	0.5058
C	-1.1398	-1.5120	-0.8758	C	3.4379	0.9157	-0.8460	H	-3.1491	2.9503	1.1596
C	-3.7411	-1.4777	0.1191	C	2.6861	2.0432	-0.8315	H	-4.4784	0.8464	1.2300
C	-2.9083	-0.3491	0.2981	C	2.9150	-0.2983	-0.2941	H	1.1244	4.1723	-0.4625
C	-1.5679	-0.3841	-0.1350	C	1.5748	-0.3555	0.1378	H	-1.1995	4.1540	0.4389
C	-2.7210	1.9986	0.8243	C	1.1657	-1.4887	0.8811	H	4.4653	0.9214	-1.2271
C	-3.4521	0.8575	0.8460	C	2.0181	-2.5475	1.0863	H	3.0971	3.0012	-1.1705
C	-1.3591	1.9850	0.3794	C	3.3215	-2.5243	0.5599	H	-0.1292	-1.5171	-1.3045
C	-0.7220	0.7721	0.0766	C	3.7670	-1.4116	-0.1111	H	1.6867	-3.4157	1.6654
C	0.6115	3.2293	-0.2414	H	-3.9200	-3.4580	-0.6952	H	3.9792	-3.3871	0.7064
C	-0.6694	3.2191	0.2240	H	-1.6301	-3.4487	-1.6578	H	4.7922	-1.3662	-0.4959

Table 3.126: Table of thermodynamic data as a function of temperature for Dibenzoc[*c,g*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.209	395.470	395.470	∞
100	92.718	319.242	682.554	-36.331	419.217	459.896	-240.220
200	181.498	409.122	523.411	-22.858	406.661	505.574	-132.040
250	233.724	455.186	505.136	-12.488	400.747	530.987	-110.941
298.15	284.870	500.734	500.734	0.000	395.470	556.562	-97.505
300	286.815	502.502	500.740	0.529	395.276	557.561	-97.078
350	337.979	550.596	504.421	16.161	390.403	585.005	-87.305
400	385.466	598.873	513.211	34.265	386.164	613.094	-80.060
450	428.492	646.804	525.397	54.633	382.489	641.685	-74.483
500	466.957	693.980	539.904	77.038	379.304	670.676	-70.064
600	531.498	785.054	573.240	127.088	374.135	729.462	-63.504
700	582.638	870.973	609.700	182.891	370.366	789.005	-58.875
800	623.776	951.555	647.451	243.283	367.826	848.988	-55.432
900	657.419	1027.031	685.479	307.397	366.352	909.221	-52.769
1000	685.308	1097.785	723.209	374.576	365.796	969.577	-50.644
1100	708.671	1164.230	760.313	444.309	365.988	1029.959	-48.908
1200	728.405	1226.762	796.604	516.189	366.801	1090.281	-47.458
1300	745.187	1285.746	831.983	589.891	368.077	1150.524	-46.228
1400	759.544	1341.509	866.405	665.146	369.704	1210.659	-45.169
1500	771.893	1394.344	899.855	741.733	371.607	1270.669	-44.248
1600	782.570	1444.510	932.342	819.469	373.676	1330.537	-43.437
1700	791.845	1492.238	963.884	898.200	375.846	1390.253	-42.716
1800	799.941	1537.732	994.511	977.799	378.052	1449.894	-42.074
1900	807.039	1581.177	1024.253	1058.155	380.267	1509.368	-41.495
2000	813.289	1622.735	1053.146	1139.178	382.442	1568.747	-40.971
2100	818.815	1662.552	1081.224	1220.789	384.512	1628.008	-40.494
2200	823.719	1700.759	1108.522	1302.921	386.477	1687.176	-40.058
2300	828.089	1737.473	1135.075	1385.515	388.329	1746.255	-39.658
2400	831.996	1772.800	1160.916	1468.523	390.009	1805.219	-39.289
2500	835.501	1806.836	1186.076	1551.901	391.527	1864.209	-38.950
2600	838.657	1839.668	1210.586	1635.612	392.852	1923.046	-38.634
2700	841.506	1871.373	1234.476	1719.622	393.986	1981.893	-38.341
2800	844.086	1902.024	1257.773	1803.904	394.909	2040.723	-38.069
2900	846.429	1931.686	1280.503	1888.432	395.595	2099.478	-37.815
3000	848.563	1960.418	1302.690	1973.183	396.079	2158.235	-37.577
3100	850.511	1988.274	1324.359	2058.138	396.298	2216.918	-37.354
3200	852.293	2015.305	1345.531	2143.279	396.286	2275.657	-37.146
3300	853.929	2041.557	1366.226	2228.592	396.026	2334.432	-36.950
3400	855.432	2067.072	1386.466	2314.061	395.497	2393.150	-36.766
3500	856.817	2091.889	1406.268	2399.674	394.701	2451.871	-36.591
3600	858.095	2116.045	1425.650	2485.421	393.657	2510.688	-36.428
3700	859.278	2139.572	1444.629	2571.290	392.338	2569.555	-36.275
3800	860.374	2162.502	1463.220	2657.273	390.722	2628.409	-36.129
3900	861.391	2184.864	1481.438	2743.362	388.844	2687.270	-35.991
4000	862.337	2206.685	1499.297	2829.549	386.689	2746.295	-35.862
4100	863.218	2227.989	1516.812	2915.827	384.228	2805.316	-35.739
4200	864.040	2248.800	1533.993	3002.191	381.485	2864.393	-35.623
4300	864.807	2269.141	1550.854	3088.633	378.446	2923.466	-35.512
4400	865.526	2289.031	1567.405	3175.150	375.120	2982.689	-35.408
4500	866.198	2308.489	1583.659	3261.737	371.517	3042.038	-35.310
4600	866.830	2327.534	1599.623	3348.389	367.597	3101.473	-35.218
4700	867.423	2346.183	1615.310	3435.102	363.370	3160.905	-35.129
4800	867.980	2364.451	1630.727	3521.872	358.875	3220.516	-35.046
4900	868.505	2382.353	1645.885	3608.697	354.052	3280.114	-34.966
5000	869.000	2399.905	1660.790	3695.572	348.976	3339.968	-34.892

3.127. Benzo[*b*]triphenylene



Other names: Dibenz[*a,c*]anthracene
1,2:3,4-Dibenzanthracene
2,3-Benztriphenylene

Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 215-58-7
Point Group: C_{2v}

Length: 13.79 Å
Width: 11.15 Å
Breadth: 3.887 Å
L/B Ratio: 1.237

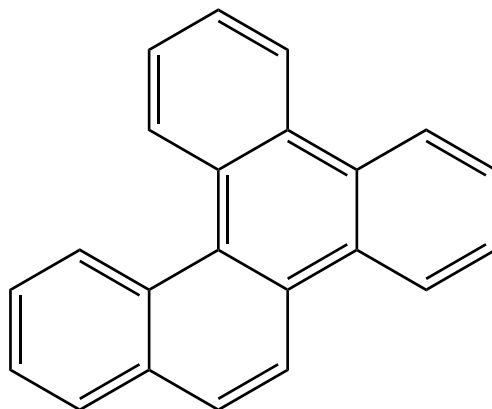
Cartesian coordinates:

C	-5.1041	0.6977	0.0000	C	3.4402	1.4538	0.0000	H	-3.9110	-2.5068	0.0000
C	-5.1009	-0.7206	0.0000	C	3.4430	2.8363	0.0000	H	-3.9222	2.4892	0.0000
C	-3.9227	-1.4111	0.0000	C	2.2341	3.5343	0.0000	H	-1.4475	-2.4994	0.0000
C	-3.9290	1.3935	0.0000	C	1.0382	2.8406	0.0000	H	-1.4587	2.4929	0.0000
C	-2.6841	0.6998	0.0000	C	2.2374	-0.7239	0.0000	H	4.3904	0.8981	0.0000
C	-2.6809	-0.7119	0.0000	C	1.0239	-1.4314	0.0000	H	4.3908	3.3843	0.0000
C	-1.4486	-1.3975	0.0000	C	1.0509	-2.8359	0.0000	H	2.2348	4.6291	0.0000
C	-1.4548	1.3910	0.0000	C	2.2499	-3.5243	0.0000	H	0.0818	3.3856	0.0000
C	-0.2493	0.7124	0.0000	C	3.4557	-2.8209	0.0000	H	0.0970	-3.3852	0.0000
C	-0.2461	-0.7135	0.0000	C	3.4467	-1.4384	0.0000	H	2.2554	-4.6190	0.0000
C	1.0175	1.4360	0.0000	H	-6.0639	1.2246	0.0000	H	4.4059	-3.3646	0.0000
C	2.2342	0.7339	0.0000	H	-6.0584	-1.2518	0.0000	H	4.3944	-0.8785	0.0000

Table 3.127: Table of thermodynamic data as a function of temperature for Benzo[*b*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-42.718	357.906	357.906	∞
100	95.529	328.869	694.075	-36.521	354.557	394.274	-205.943
200	182.332	420.133	534.428	-22.859	342.189	438.900	-114.627
250	233.682	466.284	516.165	-12.470	336.294	463.760	-96.895
298.15	284.233	511.770	511.770	0.000	331.000	488.802	-85.634
300	286.159	513.534	511.776	0.528	330.805	489.780	-85.277
350	336.930	561.495	515.447	16.117	325.889	516.675	-77.108
400	384.187	609.616	524.212	34.161	321.590	544.223	-71.067
450	427.098	657.388	536.361	54.462	317.848	572.281	-66.427
500	465.521	704.415	550.822	76.796	314.592	600.746	-62.758
600	530.099	795.228	584.055	126.704	309.281	658.503	-57.327
700	581.340	880.939	620.408	182.372	305.377	717.039	-53.505
800	622.594	961.355	658.055	242.640	302.712	776.034	-50.669
900	656.348	1036.699	695.986	306.642	301.126	835.294	-48.478
1000	684.338	1107.345	733.627	373.718	300.468	894.689	-46.733
1100	707.792	1173.702	770.649	443.358	300.567	954.119	-45.306
1200	727.607	1236.161	806.865	515.156	301.297	1013.498	-44.116
1300	744.462	1295.084	842.175	588.781	302.497	1072.805	-43.105
1400	758.884	1350.796	876.534	663.967	304.055	1132.008	-42.235
1500	771.290	1403.587	909.926	740.491	305.895	1191.091	-41.477
1600	782.019	1453.716	942.360	818.169	307.906	1250.038	-40.809
1700	791.340	1501.412	973.854	896.848	310.023	1308.835	-40.215
1800	799.477	1546.879	1004.436	976.398	312.181	1367.559	-39.685
1900	806.612	1590.300	1034.137	1056.710	314.351	1426.120	-39.206
2000	812.894	1631.836	1062.991	1137.692	316.485	1484.588	-38.773
2100	818.449	1671.635	1091.033	1219.264	318.517	1542.940	-38.378
2200	823.380	1709.825	1118.298	1301.361	320.447	1601.201	-38.017
2300	827.774	1746.525	1144.819	1383.923	322.266	1659.374	-37.685
2400	831.702	1781.839	1170.631	1466.900	323.916	1717.433	-37.378
2500	835.228	1815.863	1195.764	1550.250	325.406	1775.520	-37.097
2600	838.401	1848.685	1220.248	1633.934	326.704	1833.454	-36.834
2700	841.266	1880.381	1244.114	1717.920	327.814	1891.401	-36.591
2800	843.861	1911.023	1267.388	1802.178	328.713	1949.330	-36.364
2900	846.217	1940.677	1290.097	1886.684	329.377	2007.186	-36.153
3000	848.364	1969.402	1312.264	1971.414	329.840	2065.044	-35.955
3100	850.323	1997.252	1333.913	2056.350	330.040	2122.829	-35.769
3200	852.116	2024.277	1355.067	2141.473	330.009	2180.670	-35.595
3300	853.761	2050.524	1375.746	2226.768	329.732	2238.548	-35.433
3400	855.273	2076.034	1395.969	2312.221	329.187	2296.369	-35.279
3500	856.666	2100.847	1415.756	2397.819	328.376	2354.195	-35.134
3600	857.952	2124.998	1435.123	2483.551	327.317	2412.116	-34.998
3700	859.142	2148.521	1454.087	2569.406	325.984	2470.088	-34.871
3800	860.244	2171.448	1472.665	2655.376	324.355	2528.047	-34.750
3900	861.268	2193.807	1490.870	2741.453	322.465	2586.014	-34.635
4000	862.219	2215.624	1508.717	2827.627	320.297	2644.144	-34.528
4100	863.105	2236.926	1526.220	2913.894	317.825	2702.271	-34.427
4200	863.932	2257.735	1543.390	3000.247	315.071	2760.455	-34.331
4300	864.705	2278.072	1560.240	3086.679	312.021	2818.635	-34.239
4400	865.427	2297.960	1576.781	3173.186	308.685	2876.965	-34.153
4500	866.104	2317.416	1593.024	3259.763	305.073	2935.421	-34.073
4600	866.739	2336.459	1608.980	3346.405	301.143	2993.964	-33.997
4700	867.336	2355.106	1624.657	3433.109	296.907	3052.503	-33.924
4800	867.897	2373.372	1640.066	3519.871	292.404	3111.222	-33.856
4900	868.425	2391.273	1655.215	3606.688	287.573	3169.928	-33.791
5000	868.923	2408.823	1670.112	3693.555	282.489	3228.890	-33.731

3.128. Benzo[*g*]chrysene



Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 196-78-1
Point Group: C₁

Length: 13.73 Å
Width: 10.41 Å
Breadth: 4.927 Å
L/B Ratio: 1.319

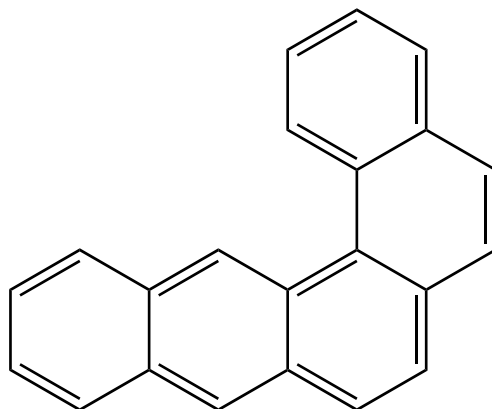
Cartesian coordinates:

C	-0.3596	-3.6517	0.4570	C	2.7811	-1.0491	-0.5408	H	-3.4254	-2.3504	-0.2276
C	0.3828	-2.4896	0.4316	C	4.1443	-0.9634	-0.6632	H	-2.3147	-4.5401	0.1793
C	-2.3409	-2.4006	-0.0455	C	4.8199	0.2240	-0.3206	H	2.4981	3.3539	0.7244
C	-1.7312	-3.6141	0.1869	C	4.1004	1.3162	0.0873	H	0.0195	3.3372	0.6067
C	-1.6000	-1.2024	-0.0404	C	-2.2860	0.0707	-0.1427	H	2.2788	-1.9831	-0.8275
C	-0.2022	-1.2422	0.1317	C	-1.5626	1.2564	0.0564	H	4.7193	-1.8183	-1.0343
C	-0.1187	1.2023	0.2017	C	-2.2551	2.4846	0.0537	H	5.9109	0.2676	-0.3985
C	0.5690	-0.0057	0.0841	C	-3.6141	2.5324	-0.1715	H	4.6051	2.2578	0.3325
C	1.9525	2.4323	0.4914	C	-4.3283	1.3499	-0.4021	H	-1.6941	3.4147	0.2292
C	0.5950	2.4135	0.4438	C	-3.6726	0.1378	-0.3834	H	-4.1390	3.4932	-0.1750
C	2.6875	1.2513	0.1851	H	0.1224	-4.6064	0.6918	H	-5.4057	1.3929	-0.5914
C	2.0048	0.0419	-0.0685	H	1.4562	-2.5457	0.6588	H	-4.2272	-0.7985	-0.5480

Table 3.128: Table of thermodynamic data as a function of temperature for Benzo[g]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-42.547	378.775	378.775	∞
100	94.668	329.916	694.809	-36.489	402.363	441.975	-230.859
200	182.226	420.834	535.200	-22.873	389.949	486.520	-127.063
250	233.839	466.990	516.922	-12.483	384.056	511.345	-106.837
298.15	284.595	512.523	512.523	0.000	378.775	536.352	-93.965
300	286.528	514.289	512.528	0.528	378.580	537.329	-93.555
350	337.464	562.319	516.205	16.140	373.687	564.184	-84.198
400	384.837	610.520	524.983	34.215	369.418	591.690	-77.265
450	427.817	658.373	537.151	54.550	365.711	619.700	-71.931
500	466.272	705.478	551.636	76.921	362.491	648.114	-67.707
600	530.834	796.428	584.922	126.904	357.255	705.757	-61.440
700	582.005	882.247	621.331	182.642	353.421	764.168	-57.022
800	623.171	962.746	659.031	242.972	350.819	823.028	-53.737
900	656.838	1038.153	697.012	307.027	349.285	882.145	-51.197
1000	684.752	1108.847	734.698	374.148	348.673	941.392	-49.172
1100	708.142	1175.240	771.761	443.827	348.810	1000.671	-47.517
1200	727.903	1237.727	808.014	515.656	349.572	1059.894	-46.135
1300	744.713	1296.672	843.357	589.309	350.800	1119.043	-44.963
1400	759.098	1352.401	877.745	664.518	352.381	1178.087	-43.954
1500	771.475	1405.206	911.165	741.062	354.241	1237.009	-43.076
1600	782.179	1455.346	943.622	818.757	356.269	1295.793	-42.302
1700	791.480	1503.051	975.138	897.451	358.401	1354.426	-41.616
1800	799.600	1548.525	1005.740	977.014	360.572	1412.986	-41.003
1900	806.720	1591.952	1035.459	1057.338	362.753	1471.382	-40.450
2000	812.991	1633.495	1064.330	1138.330	364.897	1529.684	-39.950
2100	818.535	1673.297	1092.387	1219.912	366.939	1587.870	-39.495
2200	823.458	1711.492	1119.666	1302.016	368.877	1645.965	-39.079
2300	827.844	1748.194	1146.201	1384.585	370.703	1703.971	-38.698
2400	831.766	1783.511	1172.024	1467.569	372.360	1761.863	-38.345
2500	835.285	1817.538	1197.168	1550.925	373.856	1819.782	-38.021
2600	838.453	1850.362	1221.664	1634.615	375.159	1877.549	-37.720
2700	841.314	1882.060	1245.539	1718.606	376.274	1935.328	-37.440
2800	843.905	1912.704	1268.822	1802.869	377.178	1993.089	-37.181
2900	846.259	1942.359	1291.539	1887.379	377.846	2050.777	-36.938
3000	848.402	1971.086	1313.714	1972.113	378.314	2108.466	-36.711
3100	850.358	1998.937	1335.371	2057.053	378.517	2166.083	-36.497
3200	852.149	2025.963	1356.532	2142.180	378.490	2223.756	-36.298
3300	853.792	2052.211	1377.218	2227.478	378.216	2281.465	-36.112
3400	855.302	2077.722	1397.447	2312.933	377.674	2339.118	-35.935
3500	856.693	2102.535	1417.240	2398.534	376.866	2396.774	-35.769
3600	857.978	2126.687	1436.613	2484.269	375.809	2454.527	-35.614
3700	859.166	2150.211	1455.583	2570.126	374.479	2512.330	-35.467
3800	860.267	2173.139	1474.165	2656.099	372.852	2570.120	-35.328
3900	861.289	2195.498	1492.376	2742.177	370.964	2627.918	-35.196
4000	862.239	2217.316	1510.227	2828.354	368.799	2685.879	-35.073
4100	863.125	2238.618	1527.734	2914.623	366.328	2743.837	-34.956
4200	863.950	2259.427	1544.909	3000.977	363.576	2801.852	-34.845
4300	864.722	2279.765	1561.763	3087.411	360.528	2859.862	-34.740
4400	865.444	2299.653	1578.308	3173.920	357.193	2918.023	-34.641
4500	866.120	2319.110	1594.555	3260.498	353.583	2976.309	-34.547
4600	866.754	2338.153	1610.514	3347.142	349.655	3034.682	-34.459
4700	867.350	2356.800	1626.194	3433.848	345.421	3093.053	-34.375
4800	867.911	2375.067	1641.606	3520.611	340.919	3151.602	-34.296
4900	868.438	2392.968	1656.758	3607.429	336.089	3210.138	-34.220
5000	868.936	2410.518	1671.658	3694.298	331.007	3268.931	-34.150

3.129. Dibenzo[*b,g*]phenanthrene



Other names: Naphth[1,2-*a*]anthracene
Naphtho-2',3',3,4-phenanthrene

Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 195-06-2
Point Group: C₁

Length: 14.00 Å
Width: 10.14 Å
Breadth: 4.779 Å
L/B Ratio: 1.381

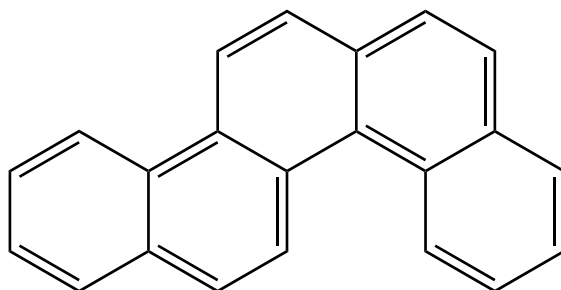
Cartesian coordinates:

C	4.4689	-2.0257	0.3678	C	-1.1256	0.6070	-0.0056	H	5.1605	1.2283	-0.4322
C	5.2201	-0.8618	0.0461	C	-1.6825	1.8832	0.0962	H	2.5236	-2.8675	0.6879
C	4.5917	0.3245	-0.1869	C	-3.0731	2.0638	0.3577	H	3.0674	2.5378	-0.4949
C	3.1092	-1.9749	0.4404	C	-3.9004	0.9918	0.4615	H	0.4678	-1.5973	0.4972
C	2.4173	-0.7485	0.1916	C	-2.0319	-0.5157	-0.0871	H	1.0640	3.8538	-0.4828
C	3.1672	0.4119	-0.1130	C	-3.4010	-0.3185	0.1996	H	-1.3762	4.0379	-0.0564
C	2.4902	1.6243	-0.3042	C	-4.3045	-1.4104	0.1797	H	-3.4553	3.0826	0.4916
C	1.0162	-0.6796	0.2391	C	-3.8777	-2.6612	-0.1831	H	-4.9609	1.1160	0.7088
C	0.3285	0.5023	-0.0199	C	-2.5354	-2.8529	-0.5613	H	-5.3527	-1.2352	0.4485
C	1.1030	1.6838	-0.2302	C	-1.6437	-1.8113	-0.5161	H	-4.5711	-3.5081	-0.1988
C	0.4513	2.9648	-0.2940	H	5.0040	-2.9624	0.5553	H	-2.2101	-3.8425	-0.8990
C	-0.8772	3.0619	-0.0766	H	6.3110	-0.9374	-0.0090	H	-0.6082	-1.9865	-0.8383

Table 3.129: Table of thermodynamic data as a function of temperature for Dibenzob[*b,g*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.259	381.456	381.456	∞
100	92.926	328.100	691.349	-36.325	405.210	445.003	-232.441
200	181.470	418.064	532.267	-22.841	392.664	489.789	-127.917
250	233.548	464.106	514.008	-12.476	386.745	514.755	-107.550
298.15	284.552	509.611	509.611	0.000	381.456	539.902	-94.587
300	286.491	511.377	509.616	0.528	381.262	540.884	-94.174
350	337.524	559.410	513.293	16.141	376.369	567.886	-84.751
400	384.911	607.620	522.072	34.219	372.105	595.536	-77.767
450	427.873	655.481	534.241	54.558	368.400	623.691	-72.395
500	466.305	702.590	548.728	76.931	365.183	652.250	-68.139
600	530.848	793.544	582.018	126.916	359.949	710.181	-61.826
700	582.037	879.367	618.430	182.656	356.117	768.880	-57.373
800	623.242	959.873	656.133	242.991	353.520	828.028	-54.064
900	656.950	1035.290	694.118	307.055	351.996	887.432	-51.504
1000	684.899	1105.998	731.808	374.190	351.396	946.965	-49.463
1100	708.315	1172.406	768.875	443.884	351.550	1006.527	-47.795
1200	728.094	1234.909	805.132	515.732	352.329	1066.033	-46.402
1300	744.914	1293.870	840.481	589.405	353.577	1125.463	-45.221
1400	759.303	1349.614	874.875	664.634	355.178	1184.786	-44.204
1500	771.680	1402.433	908.301	741.198	357.059	1243.986	-43.319
1600	782.380	1452.586	940.765	818.914	359.108	1303.047	-42.539
1700	791.676	1500.303	972.287	897.628	361.259	1361.956	-41.847
1800	799.789	1545.789	1002.894	977.210	363.449	1420.790	-41.229
1900	806.902	1589.226	1032.619	1057.552	365.649	1479.459	-40.672
2000	813.164	1630.777	1061.496	1138.562	367.811	1538.034	-40.168
2100	818.701	1670.588	1089.559	1220.161	369.870	1596.491	-39.710
2200	823.615	1708.790	1116.844	1302.281	371.824	1654.856	-39.290
2300	827.993	1745.499	1143.384	1384.866	373.665	1713.132	-38.906
2400	831.908	1780.822	1169.212	1467.864	375.337	1771.293	-38.550
2500	835.420	1814.855	1194.361	1551.234	376.846	1829.481	-38.224
2600	838.581	1847.683	1218.862	1634.937	378.163	1887.517	-37.920
2700	841.436	1879.386	1242.742	1718.940	379.290	1945.562	-37.638
2800	844.021	1910.035	1266.029	1803.215	380.206	2003.591	-37.377
2900	846.368	1939.694	1288.751	1887.736	380.886	2061.545	-37.132
3000	848.506	1968.424	1310.930	1972.482	381.364	2119.501	-36.903
3100	850.457	1996.279	1332.591	2057.431	381.578	2177.384	-36.688
3200	852.243	2023.308	1353.756	2142.567	381.560	2235.323	-36.487
3300	853.881	2049.558	1374.445	2227.875	381.295	2293.297	-36.299
3400	855.387	2075.072	1394.678	2313.339	380.762	2351.215	-36.121
3500	856.775	2099.888	1414.474	2398.948	379.962	2409.136	-35.954
3600	858.055	2124.042	1433.850	2484.691	378.913	2467.154	-35.797
3700	859.240	2147.568	1452.823	2570.556	377.591	2525.221	-35.649
3800	860.338	2170.498	1471.409	2656.536	375.971	2583.275	-35.509
3900	861.357	2192.859	1489.622	2742.621	374.090	2641.337	-35.376
4000	862.304	2214.678	1507.477	2828.805	371.931	2699.562	-35.252
4100	863.187	2235.982	1524.987	2915.080	369.467	2757.783	-35.134
4200	864.010	2256.793	1542.164	3001.440	366.721	2816.062	-35.022
4300	864.779	2277.132	1559.021	3087.880	363.679	2874.336	-34.916
4400	865.499	2297.021	1575.568	3174.394	360.350	2932.759	-34.816
4500	866.173	2316.479	1591.817	3260.978	356.745	2991.309	-34.721
4600	866.805	2335.524	1607.779	3347.628	352.822	3049.945	-34.633
4700	867.399	2354.172	1623.462	3434.338	348.593	3108.578	-34.547
4800	867.958	2372.440	1638.876	3521.106	344.096	3167.390	-34.468
4900	868.484	2390.342	1654.030	3607.929	339.270	3226.190	-34.391
5000	868.980	2407.892	1668.932	3694.802	334.192	3285.245	-34.320

3.130. Benzo[*c*]chrysene



Other names: 1,2,5,6-Dibenzophenanthrene

Formula: C₂₂H₁₄

Mass: 278.347 g/mol

CAS Number: 194-69-4

Point Group: C₁

Length: 14.39 Å

Width: 9.356 Å

Breadth: 4.791 Å

L/B Ratio: 1.538

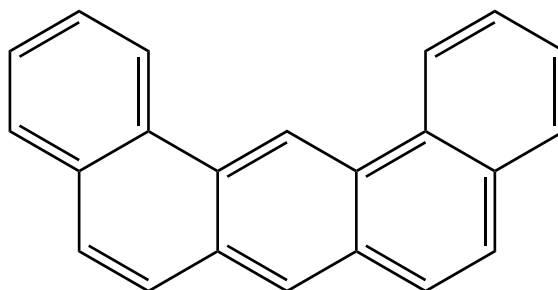
Cartesian coordinates:

C	3.4517	-2.4366	-0.5100	C	-0.2740	-0.0899	0.1243	H	5.6720	0.0113	0.2883
C	4.6820	-1.8272	-0.2152	C	-1.3761	0.7621	-0.0539	H	1.3385	-2.2166	-0.6939
C	4.7169	-0.4884	0.0893	C	-1.8009	-1.9559	0.5207	H	4.5912	2.1392	0.4890
C	2.2825	-1.7165	-0.4386	C	-0.5409	-1.4558	0.4721	H	2.5473	3.5409	0.2849
C	2.2724	-0.3513	-0.0662	C	-2.9276	-1.1299	0.2174	H	0.2300	3.7748	-0.1227
C	3.5243	0.2697	0.1314	C	-2.7199	0.2326	-0.0563	H	-2.0516	2.8073	-0.3511
C	3.6083	1.6875	0.3128	C	-3.8436	1.0488	-0.3275	H	-1.9797	-3.0004	0.8015
C	2.4926	2.4480	0.2167	C	-5.1110	0.5185	-0.3351	H	0.3026	-2.1097	0.7326
C	1.0614	0.4430	0.0374	C	-5.3112	-0.8483	-0.0673	H	-3.6812	2.1178	-0.5322
C	1.2063	1.8390	0.0510	C	-4.2378	-1.6609	0.2073	H	-5.9751	1.1559	-0.5494
C	0.0761	2.6899	-0.0870	H	3.4304	-3.4914	-0.8037	H	-6.3273	-1.2557	-0.0786
C	-1.1742	2.1619	-0.1926	H	5.6033	-2.4175	-0.2480	H	-4.3827	-2.7262	0.4196

Table 3.130: Table of thermodynamic data as a function of temperature for Benzo[*c*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-42.311	372.142	372.142	∞
100	93.291	328.629	692.103	-36.347	395.872	435.613	-227.536
200	181.560	418.756	532.962	-22.841	383.348	480.335	-125.448
250	233.548	464.807	514.704	-12.474	377.431	505.267	-105.568
298.15	284.503	510.307	510.307	0.000	372.142	530.380	-92.918
300	286.440	512.073	510.312	0.528	371.947	531.361	-92.516
350	337.459	560.097	513.988	16.138	367.052	558.327	-83.324
400	384.851	608.298	522.766	34.213	362.784	585.944	-76.515
450	427.825	656.153	534.933	54.549	359.077	614.065	-71.277
500	466.267	703.257	549.418	76.920	355.857	642.590	-67.130
600	530.816	794.205	582.704	126.901	350.620	700.456	-60.979
700	581.996	880.023	619.111	182.638	346.784	759.088	-56.643
800	623.182	960.521	656.811	242.968	344.182	818.171	-53.420
900	656.873	1035.931	694.792	307.025	342.651	877.510	-50.928
1000	684.807	1106.629	732.478	374.151	342.043	936.980	-48.942
1100	708.212	1173.028	769.541	443.836	342.187	996.480	-47.318
1200	727.984	1235.522	805.795	515.673	342.956	1055.924	-45.962
1300	744.801	1294.474	841.140	589.334	344.192	1115.293	-44.812
1400	759.190	1350.210	875.529	664.552	345.782	1174.556	-43.822
1500	771.568	1403.021	908.951	741.105	347.651	1233.697	-42.960
1600	782.271	1453.167	941.410	818.810	349.689	1292.699	-42.201
1700	791.570	1500.877	972.928	897.513	351.830	1351.550	-41.527
1800	799.688	1546.357	1003.532	977.085	354.009	1410.327	-40.926
1900	806.805	1589.789	1033.253	1057.417	356.200	1468.939	-40.383
2000	813.072	1631.335	1062.126	1138.417	358.352	1527.458	-39.892
2100	818.613	1671.142	1090.186	1220.007	360.402	1585.860	-39.445
2200	823.532	1709.339	1117.467	1302.119	362.347	1644.170	-39.037
2300	827.914	1746.045	1144.004	1384.696	364.180	1702.391	-38.662
2400	831.833	1781.365	1169.829	1467.687	365.844	1760.498	-38.315
2500	835.349	1815.395	1194.975	1551.049	367.347	1818.632	-37.997
2600	838.514	1848.221	1219.473	1634.745	368.657	1876.613	-37.701
2700	841.372	1879.921	1243.350	1718.742	369.777	1934.605	-37.426
2800	843.960	1910.567	1266.635	1803.010	370.687	1992.581	-37.171
2900	846.311	1940.225	1289.354	1887.526	371.360	2050.482	-36.932
3000	848.451	1968.953	1311.531	1972.266	371.833	2108.385	-36.709
3100	850.406	1996.805	1333.189	2057.210	372.042	2166.215	-36.500
3200	852.194	2023.833	1354.352	2142.341	372.019	2224.101	-36.304
3300	853.835	2050.082	1375.039	2227.644	371.749	2282.023	-36.121
3400	855.343	2075.594	1395.270	2313.104	371.211	2339.888	-35.947
3500	856.732	2100.409	1415.064	2398.708	370.407	2397.757	-35.784
3600	858.015	2124.562	1434.438	2484.447	369.354	2455.723	-35.631
3700	859.201	2148.087	1453.409	2570.308	368.028	2513.738	-35.487
3800	860.301	2171.015	1471.993	2656.284	366.405	2571.741	-35.350
3900	861.322	2193.376	1490.205	2742.366	364.519	2629.750	-35.221
4000	862.271	2215.194	1508.058	2828.546	362.358	2687.924	-35.100
4100	863.155	2236.497	1525.566	2914.818	359.890	2746.094	-34.985
4200	863.979	2257.307	1542.742	3001.175	357.140	2804.321	-34.876
4300	864.749	2277.646	1559.597	3087.612	354.095	2862.543	-34.772
4400	865.470	2297.535	1576.143	3174.123	350.764	2920.916	-34.675
4500	866.145	2316.992	1592.391	3260.704	347.156	2979.414	-34.583
4600	866.779	2336.036	1608.351	3347.351	343.230	3037.999	-34.497
4700	867.374	2354.683	1624.033	3434.059	338.998	3096.581	-34.414
4800	867.933	2372.950	1639.445	3520.824	334.499	3155.342	-34.336
4900	868.460	2390.852	1654.598	3607.644	329.671	3214.090	-34.262
5000	868.957	2408.402	1669.499	3694.515	324.591	3273.094	-34.193

3.131. Dibenz[*a,j*]anthracene



Other names: 1,2,7,8-Dibenzanthracene
3,4,5,6-Dibenzanthracene
Dibenzo-1,2,7,8-anthracene

Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 224-41-9
Point Group: C_{2v}

Length: 14.21 Å
Width: 9.487 Å
Breadth: 3.884 Å
L/B Ratio: 1.497

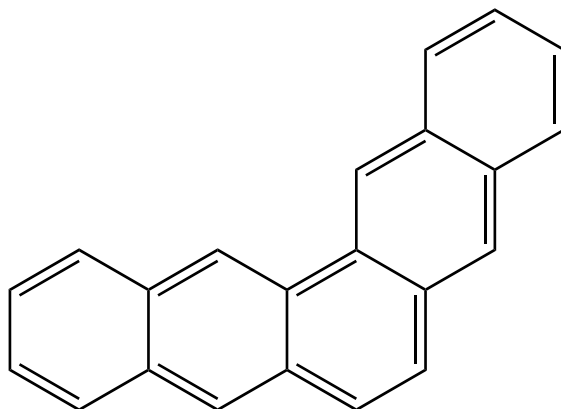
Cartesian coordinates:

C	4.9475	-1.7871	0.0000	C	-1.2162	0.2412	0.0000	H	1.5914	-2.4287	0.0000
C	4.9149	-0.4088	0.0000	C	-1.2159	1.6567	0.0000	H	3.7892	-3.6151	0.0000
C	2.5387	-1.8678	0.0000	C	-2.4695	2.3674	0.0000	H	4.5937	2.2551	0.0000
C	3.7523	-2.5209	0.0000	C	-3.6460	1.7025	0.0000	H	2.4298	3.4701	0.0000
C	2.4830	-0.4600	0.0000	C	-2.4817	-0.4671	0.0000	H	-0.0049	3.4465	0.0000
C	3.6820	0.2732	0.0000	C	-3.6828	0.2627	0.0000	H	0.0022	-1.5491	0.0000
C	3.6411	1.7129	0.0000	C	-4.9137	-0.4229	0.0000	H	-2.4398	3.4631	0.0000
C	2.4627	2.3744	0.0000	C	-4.9423	-1.8012	0.0000	H	-4.6002	2.2419	0.0000
C	1.2155	0.2447	0.0000	C	-3.7450	-2.5316	0.0000	H	-5.8471	0.1514	0.0000
C	1.2112	1.6602	0.0000	C	-2.5333	-1.8750	0.0000	H	-5.8994	-2.3331	0.0000
C	-0.0034	2.3493	0.0000	H	5.9061	-2.3162	0.0000	H	-3.7788	-3.6259	0.0000
C	0.0006	-0.4420	0.0000	H	5.8466	0.1682	0.0000	H	-1.5844	-2.4332	0.0000

Table 3.131: Table of thermodynamic data as a function of temperature for Dibenz[*a,j*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-42.412	346.233	346.233	∞
100	93.987	325.495	689.175	-36.368	369.943	409.997	-214.156
200	181.643	415.906	530.028	-22.824	357.457	455.013	-118.835
250	233.368	461.947	511.787	-12.460	351.537	480.087	-100.307
298.15	284.088	507.395	507.395	0.000	346.233	505.339	-88.532
300	286.018	509.158	507.400	0.527	346.037	506.326	-88.157
350	336.833	557.101	511.071	16.111	341.116	533.440	-79.610
400	384.076	605.209	519.832	34.151	336.813	561.208	-73.285
450	426.957	652.966	531.977	54.445	333.064	589.487	-68.424
500	465.355	699.977	546.434	76.771	329.800	618.173	-64.579
600	529.921	790.758	579.656	126.661	324.471	676.375	-58.883
700	581.191	876.444	615.997	182.313	320.551	735.360	-54.872
800	622.491	956.842	653.632	242.568	317.873	794.806	-51.894
900	656.293	1032.177	691.553	306.562	316.279	854.517	-49.594
1000	684.326	1102.820	729.185	373.635	315.618	914.364	-47.761
1100	707.814	1169.177	766.199	443.276	315.718	974.248	-46.262
1200	727.655	1231.639	802.408	515.077	316.451	1034.078	-45.011
1300	744.528	1290.567	837.714	588.708	317.657	1093.837	-43.950
1400	758.961	1346.284	872.069	663.901	319.222	1153.492	-43.036
1500	771.376	1399.081	905.459	740.433	321.070	1213.026	-42.240
1600	782.108	1449.215	937.890	818.120	323.090	1272.423	-41.539
1700	791.431	1496.916	969.382	896.808	325.216	1331.670	-40.916
1800	799.568	1542.389	999.963	976.367	327.383	1390.843	-40.360
1900	806.702	1585.815	1029.663	1056.688	329.562	1449.853	-39.858
2000	812.982	1627.356	1058.517	1137.679	331.705	1508.769	-39.404
2100	818.535	1667.159	1086.558	1219.260	333.746	1567.569	-38.990
2200	823.463	1705.353	1113.823	1301.365	335.684	1626.277	-38.612
2300	827.853	1742.056	1140.345	1383.935	337.511	1684.897	-38.264
2400	831.779	1777.373	1166.157	1466.920	339.169	1743.403	-37.943
2500	835.300	1811.401	1191.290	1550.277	340.666	1801.936	-37.649
2600	838.470	1844.225	1215.775	1633.969	341.972	1860.317	-37.373
2700	841.333	1875.924	1239.642	1717.961	343.088	1918.709	-37.119
2800	843.924	1906.569	1262.916	1802.226	343.994	1977.084	-36.882
2900	846.278	1936.225	1285.625	1886.738	344.664	2035.385	-36.660
3000	848.422	1964.952	1307.793	1971.475	345.134	2093.688	-36.454
3100	850.378	1992.803	1329.443	2056.416	345.339	2151.918	-36.259
3200	852.169	2019.831	1350.598	2141.545	345.314	2210.205	-36.077
3300	853.811	2046.079	1371.277	2226.845	345.042	2268.527	-35.907
3400	855.321	2071.590	1391.501	2312.303	344.502	2326.793	-35.746
3500	856.712	2096.404	1411.288	2397.905	343.695	2385.062	-35.594
3600	857.996	2120.557	1430.656	2483.642	342.641	2443.428	-35.452
3700	859.184	2144.081	1449.622	2569.501	341.312	2501.844	-35.319
3800	860.285	2167.009	1468.200	2655.475	339.688	2560.247	-35.192
3900	861.306	2189.369	1486.406	2741.556	337.801	2618.658	-35.072
4000	862.256	2211.187	1504.254	2827.734	335.637	2677.232	-34.960
4100	863.141	2232.490	1521.757	2914.005	333.169	2735.803	-34.854
4200	863.967	2253.299	1538.928	3000.361	330.418	2794.430	-34.753
4300	864.738	2273.638	1555.778	3086.796	327.371	2853.053	-34.657
4400	865.459	2293.526	1572.320	3173.306	324.039	2911.827	-34.567
4500	866.135	2312.983	1588.564	3259.887	320.430	2970.726	-34.483
4600	866.769	2332.027	1604.520	3346.532	316.503	3029.712	-34.403
4700	867.364	2350.674	1620.198	3433.239	312.270	3088.695	-34.326
4800	867.924	2368.941	1635.607	3520.004	307.770	3147.856	-34.255
4900	868.452	2386.843	1650.756	3606.823	302.941	3207.006	-34.186
5000	868.949	2404.393	1665.654	3693.693	297.860	3266.411	-34.123

3.132. Pentaphene



Other names: Dibenzo[*b,h*]phenanthrene
2,3,6,7-Dibenzophenanthrene
 β,β' -Dibenzophenanthrene
Naphtho-2',3',1,2-anthracene

Formula: $C_{22}H_{14}$
Mass: 278.347 g/mol
CAS Number: 222-93-5
Point Group: C_{2v}

Length: 15.91 Å
Width: 9.164 Å
Breadth: 3.884 Å
L/B Ratio: 1.736

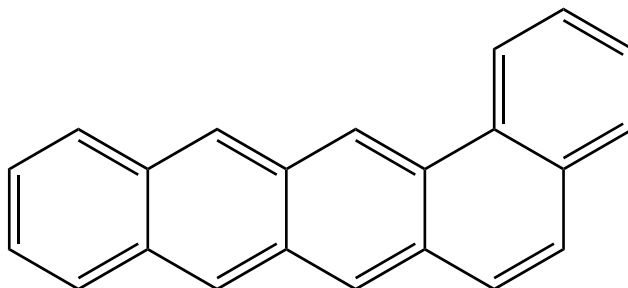
Cartesian coordinates:

C	4.9683	-2.0704	0.0000	C	-0.7291	0.2922	0.0000	H	5.4981	1.3075	0.0000
C	5.6603	-0.8322	0.0000	C	-1.4239	1.5369	0.0000	H	3.0607	-3.0532	0.0000
C	4.9713	0.3466	0.0000	C	-2.8068	1.5588	0.0000	H	3.3508	2.5063	0.0000
C	3.6033	-2.1011	0.0000	C	-1.4486	-0.8890	0.0000	H	0.9038	-1.8522	0.0000
C	2.8564	-0.8869	0.0000	C	-2.8588	-0.8792	0.0000	H	1.2431	3.7095	0.0000
C	3.5457	0.3469	0.0000	C	-3.5447	0.3564	0.0000	H	-1.2332	3.7128	0.0000
C	2.8110	1.5512	0.0000	C	-4.9703	0.3600	0.0000	H	-3.3440	2.5153	0.0000
C	1.4462	-0.8929	0.0000	C	-5.6625	-0.8168	0.0000	H	-0.9088	-1.8498	0.0000
C	0.7298	0.2902	0.0000	C	-4.9738	-2.0569	0.0000	H	-5.4944	1.3224	0.0000
C	1.4280	1.5331	0.0000	C	-3.6089	-2.0913	0.0000	H	-6.7574	-0.8199	0.0000
C	0.6767	2.7708	0.0000	H	5.5471	-2.9999	0.0000	H	-5.5551	-2.9848	0.0000
C	-0.6693	2.7726	0.0000	H	6.7552	-0.8382	0.0000	H	-3.0689	-3.0448	0.0000

Table 3.132: Table of thermodynamic data as a function of temperature for Pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-42.424	359.293	359.293	∞
100	93.519	323.871	688.369	-36.450	382.922	423.138	-221.020
200	182.095	414.287	528.788	-22.900	370.441	468.321	-122.310
250	234.155	460.465	510.484	-12.505	364.553	493.473	-103.104
298.15	285.148	506.076	506.076	0.000	359.293	518.793	-90.888
300	287.086	507.846	506.082	0.529	359.100	519.782	-90.500
350	338.091	555.969	509.766	16.171	354.237	546.957	-81.627
400	385.434	604.252	518.560	34.277	349.999	574.778	-75.057
450	428.348	652.172	530.749	54.640	346.320	603.100	-70.005
500	466.734	699.329	545.257	77.036	343.125	631.822	-66.005
600	531.209	790.355	578.588	127.060	337.930	690.077	-60.075
700	582.362	876.230	615.038	182.834	334.133	749.091	-55.897
800	623.548	956.777	652.776	243.201	331.567	808.551	-52.792
900	657.248	1032.230	690.791	307.295	330.073	868.262	-50.392
1000	685.190	1102.969	728.510	374.459	329.503	928.100	-48.478
1100	708.598	1169.405	765.602	444.182	329.685	987.964	-46.914
1200	728.367	1231.932	801.884	516.058	330.492	1047.768	-45.607
1300	745.176	1290.914	837.255	589.757	331.767	1107.495	-44.499
1400	759.553	1346.677	871.669	665.012	333.393	1167.113	-43.545
1500	771.917	1399.513	905.113	741.601	335.298	1226.606	-42.713
1600	782.604	1449.681	937.594	819.340	337.370	1285.958	-41.981
1700	791.887	1497.411	969.132	898.075	339.543	1345.156	-41.331
1800	799.988	1542.908	999.754	977.678	341.754	1404.279	-40.750
1900	807.089	1586.356	1029.493	1058.039	343.974	1463.235	-40.226
2000	813.340	1627.916	1058.383	1139.067	346.154	1522.097	-39.752
2100	818.866	1667.736	1086.458	1220.683	348.229	1580.839	-39.320
2200	823.770	1705.945	1113.754	1302.820	350.199	1639.489	-38.926
2300	828.139	1742.661	1140.305	1385.419	352.056	1698.050	-38.563
2400	832.045	1777.991	1166.144	1468.432	353.742	1756.494	-38.228
2500	835.549	1812.029	1191.303	1551.815	355.264	1814.965	-37.921
2600	838.703	1844.862	1215.812	1635.530	356.594	1873.283	-37.634
2700	841.551	1876.569	1239.701	1719.545	357.733	1931.611	-37.368
2800	844.129	1907.222	1262.996	1803.832	358.660	1989.921	-37.122
2900	846.471	1936.885	1285.725	1888.363	359.350	2048.156	-36.891
3000	848.603	1965.618	1307.912	1973.119	359.838	2106.393	-36.675
3100	850.550	1993.476	1329.580	2058.078	360.061	2164.556	-36.472
3200	852.331	2020.508	1350.751	2143.223	360.053	2222.775	-36.282
3300	853.964	2046.761	1371.446	2228.539	359.797	2281.029	-36.105
3400	855.466	2072.277	1391.686	2314.012	359.271	2339.226	-35.937
3500	856.850	2097.095	1411.487	2399.628	358.479	2397.427	-35.779
3600	858.127	2121.252	1430.869	2485.378	357.438	2455.724	-35.631
3700	859.308	2144.780	1449.847	2571.251	356.122	2514.070	-35.492
3800	860.403	2167.711	1468.438	2657.237	354.509	2572.403	-35.359
3900	861.419	2190.073	1486.656	2743.329	352.634	2630.743	-35.234
4000	862.364	2211.895	1504.515	2829.518	350.482	2689.247	-35.117
4100	863.244	2233.200	1522.029	2915.799	348.024	2747.747	-35.006
4200	864.065	2254.012	1539.211	3002.165	345.283	2806.303	-34.901
4300	864.831	2274.353	1556.071	3088.610	342.246	2864.855	-34.800
4400	865.549	2294.243	1572.623	3175.130	338.922	2923.557	-34.706
4500	866.221	2313.702	1588.876	3261.719	335.322	2982.384	-34.618
4600	866.851	2332.748	1604.841	3348.373	331.404	3041.298	-34.534
4700	867.444	2351.397	1620.527	3435.088	327.179	3100.209	-34.454
4800	868.001	2369.665	1635.944	3521.860	322.687	3159.298	-34.379
4900	868.525	2387.568	1651.102	3608.687	317.865	3218.375	-34.308
5000	869.019	2405.120	1666.007	3695.564	312.792	3277.707	-34.241

3.133. Benzo[*a*]naphthacene



Other names: 1,2,6,7-Dibenzanthracene
Naphtho-2',3',2,3-phenanthrene

Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 226-88-0
Point Group: C_s

Length: 16.05 Å
Width: 8.990 Å
Breadth: 3.884 Å
L/B Ratio: 1.785

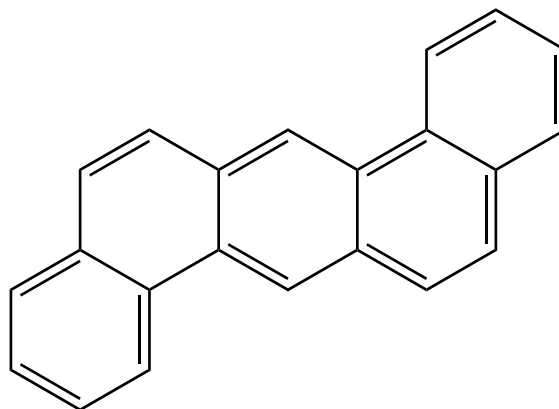
Cartesian coordinates:

C	5.6819	-1.2680	0.0000	C	-1.4933	0.0212	0.0000	H	5.0929	2.1054	0.0000
C	5.9356	0.1374	0.0000	C	-1.2360	1.4323	0.0000	H	4.2043	-2.8171	0.0000
C	4.9083	1.0251	0.0000	C	-2.3527	2.3528	0.0000	H	2.6758	2.5427	0.0000
C	4.4090	-1.7405	0.0000	C	-3.6249	1.9094	0.0000	H	1.7865	-2.3814	0.0000
C	3.2935	-0.8357	0.0000	C	-2.8747	-0.4411	0.0000	H	0.2610	2.9762	0.0000
C	3.5468	0.5676	0.0000	C	-3.9226	0.4950	0.0000	H	-0.6390	-1.9458	0.0000
C	2.4830	1.4628	0.0000	C	-5.2548	0.0488	0.0000	H	-2.1282	3.4258	0.0000
C	1.9837	-1.3023	0.0000	C	-5.5370	-1.3042	0.0000	H	-4.4686	2.6093	0.0000
C	0.9054	-0.4022	0.0000	C	-4.4961	-2.2384	0.0000	H	-6.0685	0.7829	0.0000
C	1.1578	0.9969	0.0000	C	-3.1818	-1.8123	0.0000	H	-6.5760	-1.6494	0.0000
C	0.0591	1.8978	0.0000	H	6.5356	-1.9536	0.0000	H	-4.7264	-3.3087	0.0000
C	-0.4381	-0.8621	0.0000	H	6.9751	0.4812	0.0000	H	-2.3529	-2.5367	0.0000

Table 3.133: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-42.517	372.801	372.801	∞
100	93.950	331.456	696.230	-36.477	396.402	435.859	-227.665
200	182.239	422.050	536.569	-22.904	383.945	480.273	-125.432
250	234.193	468.250	518.264	-12.503	378.062	505.036	-105.519
298.15	285.056	513.857	513.857	0.000	372.801	529.981	-92.848
300	286.989	515.626	513.862	0.529	372.607	530.955	-92.446
350	337.869	563.725	517.545	16.163	367.736	557.742	-83.237
400	385.118	611.971	526.334	34.255	363.485	585.176	-76.415
450	427.971	659.850	538.515	54.601	359.788	613.113	-71.167
500	466.325	706.965	553.012	76.977	356.574	641.453	-67.011
600	530.788	797.915	586.317	126.959	351.337	698.947	-60.847
700	581.964	883.727	622.738	182.692	347.498	757.209	-56.502
800	623.186	964.223	660.447	243.021	344.894	815.922	-53.273
900	656.922	1039.636	698.435	307.081	343.366	874.891	-50.776
1000	684.899	1110.342	736.128	374.214	342.765	933.989	-48.786
1100	708.338	1176.751	773.197	443.909	342.919	993.117	-47.158
1200	728.135	1239.257	809.457	515.760	343.702	1052.188	-45.800
1300	744.968	1298.222	844.808	589.438	344.955	1111.183	-44.647
1400	759.366	1353.970	879.204	664.673	346.562	1170.071	-43.655
1500	771.748	1406.794	912.631	741.244	348.449	1228.835	-42.791
1600	782.451	1456.951	945.097	818.967	350.505	1287.460	-42.030
1700	791.748	1504.672	976.621	897.687	352.663	1345.932	-41.355
1800	799.861	1550.162	1007.231	977.277	354.861	1404.329	-40.752
1900	806.972	1593.603	1036.958	1057.626	357.068	1462.560	-40.208
2000	813.233	1635.158	1065.837	1138.643	359.237	1520.697	-39.716
2100	818.768	1674.972	1093.902	1220.249	361.303	1578.716	-39.268
2200	823.680	1713.177	1121.188	1302.376	363.263	1636.642	-38.858
2300	828.055	1749.890	1147.730	1384.967	365.111	1694.480	-38.482
2400	831.967	1785.215	1173.561	1467.971	366.788	1752.202	-38.135
2500	835.477	1819.250	1198.712	1551.347	368.304	1809.950	-37.816
2600	838.636	1852.081	1223.214	1635.055	369.626	1867.546	-37.519
2700	841.488	1883.786	1247.096	1719.064	370.759	1925.152	-37.244
2800	844.070	1914.436	1270.385	1803.344	371.680	1982.740	-36.988
2900	846.416	1944.097	1293.108	1887.870	372.364	2040.255	-36.748
3000	848.551	1972.829	1315.289	1972.620	372.847	2097.770	-36.525
3100	850.501	2000.685	1336.951	2057.574	373.065	2155.212	-36.314
3200	852.284	2027.716	1358.117	2142.714	373.051	2212.710	-36.118
3300	853.921	2053.967	1378.808	2228.026	372.791	2270.244	-35.934
3400	855.425	2079.482	1399.042	2313.494	372.261	2327.720	-35.760
3500	856.811	2104.299	1418.840	2399.107	371.465	2385.201	-35.596
3600	858.090	2128.454	1438.217	2484.853	370.420	2442.777	-35.443
3700	859.273	2151.981	1457.192	2570.722	369.101	2500.403	-35.299
3800	860.370	2174.911	1475.779	2656.705	367.485	2558.016	-35.162
3900	861.387	2197.273	1493.993	2742.793	365.606	2615.636	-35.032
4000	862.334	2219.094	1511.849	2828.980	363.451	2673.420	-34.911
4100	863.215	2240.398	1529.359	2915.258	360.990	2731.200	-34.795
4200	864.037	2261.209	1546.538	3001.621	358.246	2789.037	-34.686
4300	864.805	2281.550	1563.395	3088.063	355.206	2846.869	-34.582
4400	865.524	2301.439	1579.944	3174.580	351.880	2904.851	-34.484
4500	866.197	2320.898	1596.194	3261.166	348.277	2962.959	-34.392
4600	866.828	2339.943	1612.156	3347.818	344.357	3021.153	-34.306
4700	867.421	2358.591	1627.840	3434.531	340.130	3079.344	-34.222
4800	867.979	2376.859	1643.255	3521.301	335.635	3137.714	-34.145
4900	868.504	2394.762	1658.410	3608.126	330.812	3196.072	-34.070
5000	869.000	2412.313	1673.313	3695.001	325.736	3254.685	-34.001

3.134. Dibenz[*a,h*]anthracene



Other names: 1,2:5,6-Benz[*a*]anthracene
 1,2:5,6-Benzanthracene
 1,2,5,6-Dibenzoanthracene

Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 53-70-3
Point Group: C_{2h}

Length: 15.68 Å
Width: 8.711 Å
Breadth: 3.885 Å
L/B Ratio: 1.800

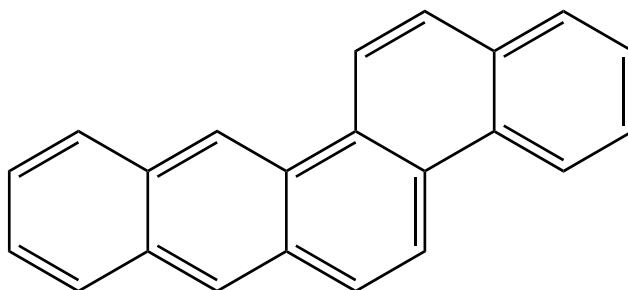
Cartesian coordinates:

C	5.0480	-0.7386	0.0000	C	-1.3993	-0.1582	0.0000	H	5.3137	2.6489	0.0000
C	5.6348	0.5088	0.0000	C	-0.8249	1.1356	0.0000	H	2.8246	2.4520	0.0000
C	4.8379	1.6628	0.0000	C	-1.6811	2.2945	0.0000	H	1.2084	-3.2834	0.0000
C	3.4639	1.5558	0.0000	C	-3.0263	2.1650	0.0000	H	3.6789	-3.0457	0.0000
C	3.6446	-0.8643	0.0000	C	-2.8438	-0.2907	0.0000	H	1.0208	2.2797	0.0000
C	2.8438	0.2907	0.0000	C	-3.6446	0.8643	0.0000	H	-1.0208	-2.2797	0.0000
C	1.6811	-2.2944	0.0000	C	-5.0480	0.7386	0.0000	H	-1.2085	3.2834	0.0000
C	3.0262	-2.1650	0.0000	C	-5.6348	-0.5089	0.0000	H	-3.6790	3.0457	0.0000
C	0.8249	-1.1355	0.0000	C	-4.8378	-1.6628	0.0000	H	-5.6671	1.6429	0.0000
C	1.3993	0.1582	0.0000	C	-3.4639	-1.5558	0.0000	H	-6.7254	-0.6055	0.0000
C	0.5638	1.2767	0.0000	H	5.6671	-1.6430	0.0000	H	-5.3136	-2.6489	0.0000
C	-0.5638	-1.2767	0.0000	H	6.7254	0.6054	0.0000	H	-2.8246	-2.4520	0.0000

Table 3.134: Table of thermodynamic data as a function of temperature for Dibenz[*a,h*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-42.467	344.936	344.936	∞
100	94.289	326.510	690.357	-36.385	351.693	391.646	-204.570
200	181.706	417.048	531.169	-22.824	339.224	436.552	-114.013
250	233.358	463.095	512.928	-12.458	333.306	461.569	-96.438
298.15	284.037	508.537	508.537	0.000	328.000	486.766	-85.278
300	285.965	510.300	508.543	0.527	327.804	487.750	-84.923
350	336.760	558.233	512.212	16.107	322.879	514.807	-76.829
400	383.997	606.331	520.972	34.143	318.572	542.519	-70.844
450	426.880	654.079	533.114	54.434	314.820	570.742	-66.249
500	465.284	701.082	547.569	76.757	311.553	599.373	-62.615
600	529.864	791.851	580.784	126.640	306.217	657.465	-57.236
700	581.147	877.529	617.120	182.287	302.292	716.341	-53.453
800	622.459	957.923	654.750	242.538	299.610	775.679	-50.646
900	656.270	1033.254	692.666	306.529	298.013	835.282	-48.477
1000	684.310	1103.895	730.294	373.601	297.351	895.022	-46.750
1100	707.804	1170.251	767.305	443.240	297.449	954.797	-45.339
1200	727.648	1232.712	803.512	515.040	298.181	1014.521	-44.160
1300	744.524	1291.639	838.816	588.671	299.387	1074.172	-43.160
1400	758.960	1347.357	873.168	663.864	300.952	1133.720	-42.299
1500	771.376	1400.153	906.556	740.396	302.800	1193.147	-41.548
1600	782.109	1450.288	938.986	818.083	304.820	1252.436	-40.887
1700	791.433	1497.989	970.477	896.770	306.945	1311.576	-40.299
1800	799.570	1543.462	1001.056	976.330	309.113	1370.642	-39.774
1900	806.704	1586.887	1030.755	1056.651	311.292	1429.544	-39.300
2000	812.985	1628.429	1059.608	1137.642	313.435	1488.353	-38.871
2100	818.538	1668.232	1087.649	1219.224	315.477	1547.046	-38.480
2200	823.466	1706.426	1114.913	1301.329	317.415	1605.647	-38.122
2300	827.856	1743.129	1141.434	1383.899	319.242	1664.160	-37.793
2400	831.781	1778.447	1167.245	1466.885	320.901	1722.558	-37.490
2500	835.303	1812.475	1192.378	1550.242	322.398	1780.984	-37.211
2600	838.473	1845.299	1216.863	1633.933	323.703	1839.257	-36.950
2700	841.335	1876.997	1240.728	1717.926	324.820	1897.542	-36.709
2800	843.927	1907.642	1264.003	1802.192	325.727	1955.810	-36.485
2900	846.281	1937.299	1286.711	1886.704	326.397	2014.003	-36.275
3000	848.424	1966.026	1308.879	1971.441	326.867	2072.199	-36.079
3100	850.381	1993.878	1330.529	2056.382	327.072	2130.322	-35.895
3200	852.171	2020.905	1351.683	2141.511	327.047	2188.501	-35.723
3300	853.813	2047.153	1372.362	2226.812	326.776	2246.715	-35.562
3400	855.323	2072.665	1392.585	2312.270	326.236	2304.874	-35.409
3500	856.714	2097.479	1412.372	2397.872	325.429	2363.036	-35.266
3600	857.998	2121.631	1431.740	2483.609	324.375	2421.294	-35.131
3700	859.186	2145.156	1450.705	2569.469	323.047	2479.603	-35.005
3800	860.287	2168.084	1469.283	2655.443	321.422	2537.898	-34.885
3900	861.308	2190.444	1487.489	2741.524	319.536	2596.201	-34.771
4000	862.258	2212.262	1505.336	2827.702	317.372	2654.668	-34.666
4100	863.143	2233.564	1522.839	2913.973	314.904	2713.131	-34.565
4200	863.968	2254.374	1540.010	3000.329	312.153	2771.651	-34.470
4300	864.739	2274.713	1556.861	3086.765	309.107	2830.167	-34.379
4400	865.460	2294.601	1573.402	3173.275	305.774	2888.833	-34.294
4500	866.136	2314.058	1589.646	3259.855	302.165	2947.625	-34.214
4600	866.770	2333.102	1605.602	3346.501	298.239	3006.503	-34.139
4700	867.366	2351.749	1621.279	3433.208	294.006	3065.378	-34.067
4800	867.926	2370.016	1636.689	3519.973	289.506	3124.433	-34.000
4900	868.453	2387.918	1651.838	3606.792	284.677	3183.474	-33.936
5000	868.950	2405.468	1666.735	3693.663	279.597	3242.772	-33.876

3.135. Benzo[*b*]chrysene



Other names: Benzo[*c*]tetraphene
 2,3-Benzochrysene
 3,4-Benzotetraphene
 Dibenzo[*a,h*]phenanthrene
 2,3:7,8-Dibenzophenanthrene
 Naphth[2,1-*a*]anthracene
 Naphtho-2',3',1,2-phenanthrene

Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 214-17-5
Point Group: C_s

Length: 16.10 Å
Width: 8.723 Å
Breadth: 3.884 Å
L/B Ratio: 1.846

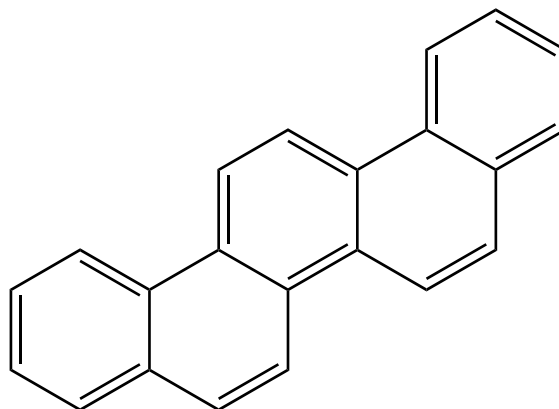
Cartesian coordinates:

C	5.4411	-1.3473	0.0000	C	-0.6503	-0.3965	0.0000	H	5.1556	2.0621	0.0000
C	5.8199	0.0237	0.0000	C	-1.6064	0.6156	0.0000	H	3.8248	-2.7556	0.0000
C	4.8732	1.0033	0.0000	C	-2.3869	-2.0923	0.0000	H	2.7834	2.7144	0.0000
C	4.1258	-1.7019	0.0000	C	-1.0674	-1.7610	0.0000	H	1.4492	-2.1031	0.0000
C	3.1061	-0.6995	0.0000	C	-3.3882	-1.0756	0.0000	H	0.4384	3.3745	0.0000
C	3.4836	0.6665	0.0000	C	-3.0040	0.2789	0.0000	H	-1.9720	2.7619	0.0000
C	2.4907	1.6571	0.0000	C	-4.0134	1.2744	0.0000	H	-2.7029	-3.1417	0.0000
C	1.7464	-1.0421	0.0000	C	-5.3399	0.9271	0.0000	H	-0.2874	-2.5380	0.0000
C	0.7604	-0.0606	0.0000	C	-5.7201	-0.4308	0.0000	H	-3.7047	2.3309	0.0000
C	1.1439	1.3097	0.0000	C	-4.7642	-1.4143	0.0000	H	-6.1150	1.7004	0.0000
C	0.1238	2.3246	0.0000	H	6.2261	-2.1106	0.0000	H	-6.7839	-0.6895	0.0000
C	-1.1865	1.9907	0.0000	H	6.8854	0.2758	0.0000	H	-5.0504	-2.4722	0.0000

Table 3.135: Table of thermodynamic data as a function of temperature for Benzo[*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-42.480	356.901	356.901	∞
100	93.984	331.688	696.014	-36.433	380.547	419.981	-219.371
200	181.962	422.196	536.562	-22.873	368.076	464.374	-121.280
250	233.874	468.329	518.281	-12.488	362.177	489.132	-102.196
298.15	284.740	513.879	513.879	0.000	356.901	514.074	-90.062
300	286.674	515.647	513.885	0.529	356.707	515.048	-89.676
350	337.580	563.698	517.563	16.147	351.820	541.836	-80.863
400	384.863	611.909	526.345	34.226	347.556	569.272	-74.338
450	427.746	659.760	538.516	54.560	343.847	597.212	-69.321
500	466.121	706.852	553.002	76.925	340.622	625.558	-65.350
600	530.604	797.766	586.287	126.888	335.366	683.065	-59.465
700	581.776	883.550	622.689	182.602	331.509	741.343	-55.319
800	622.986	964.021	660.381	242.912	328.885	800.075	-52.238
900	656.709	1039.409	698.352	306.951	327.336	859.065	-49.858
1000	684.676	1110.092	736.029	374.062	326.714	918.188	-47.960
1100	708.110	1176.479	773.084	443.735	326.845	977.342	-46.409
1200	727.907	1238.966	809.329	515.563	327.606	1036.441	-45.114
1300	744.744	1297.912	844.667	589.218	328.835	1095.466	-44.015
1400	759.148	1353.644	879.050	664.431	330.420	1154.386	-43.070
1500	771.538	1406.453	912.466	740.981	332.286	1213.184	-42.246
1600	782.251	1456.597	944.920	818.683	334.321	1271.843	-41.521
1700	791.557	1504.306	976.433	897.384	336.460	1330.351	-40.876
1800	799.680	1549.786	1007.033	976.955	338.639	1388.785	-40.301
1900	806.801	1593.217	1036.750	1057.287	340.829	1447.054	-39.781
2000	813.072	1634.763	1065.620	1138.287	342.981	1505.230	-39.312
2100	818.615	1674.570	1093.676	1219.877	345.031	1563.289	-38.884
2200	823.536	1712.768	1120.955	1301.989	346.976	1621.256	-38.493
2300	827.920	1749.474	1147.489	1384.566	348.810	1679.135	-38.134
2400	831.840	1784.794	1173.312	1467.558	350.475	1736.899	-37.802
2500	835.356	1818.824	1198.456	1550.921	351.978	1794.689	-37.497
2600	838.522	1851.650	1222.951	1634.617	353.288	1852.328	-37.213
2700	841.380	1883.351	1246.827	1718.615	354.410	1909.977	-36.950
2800	843.969	1913.997	1270.110	1802.884	355.320	1967.609	-36.705
2900	846.319	1943.655	1292.827	1887.400	355.995	2025.168	-36.476
3000	848.460	1972.383	1315.003	1972.141	356.468	2082.727	-36.263
3100	850.414	2000.236	1336.660	2057.086	356.677	2140.214	-36.062
3200	852.202	2027.265	1357.821	2142.218	356.655	2197.757	-35.874
3300	853.843	2053.514	1378.507	2227.522	356.387	2255.336	-35.698
3400	855.351	2079.026	1398.737	2312.982	355.850	2312.858	-35.532
3500	856.740	2103.841	1418.530	2398.588	355.046	2370.384	-35.375
3600	858.023	2127.994	1437.904	2484.327	353.994	2428.007	-35.229
3700	859.209	2151.520	1456.874	2570.189	352.668	2485.679	-35.091
3800	860.308	2174.448	1475.457	2656.166	351.046	2543.338	-34.960
3900	861.329	2196.808	1493.668	2742.248	349.161	2601.004	-34.836
4000	862.277	2218.627	1511.520	2828.429	347.000	2658.835	-34.720
4100	863.161	2239.930	1529.027	2914.702	344.534	2716.661	-34.610
4200	863.986	2260.740	1546.202	3001.059	341.784	2774.545	-34.506
4300	864.756	2281.080	1563.057	3087.497	338.740	2832.424	-34.406
4400	865.476	2300.968	1579.603	3174.009	335.409	2890.453	-34.313
4500	866.151	2320.426	1595.850	3260.591	331.802	2948.608	-34.226
4600	866.785	2339.470	1611.809	3347.238	327.877	3006.850	-34.143
4700	867.379	2358.117	1627.490	3433.946	323.645	3065.088	-34.064
4800	867.939	2376.385	1642.903	3520.712	319.147	3123.506	-33.990
4900	868.466	2394.286	1658.055	3607.533	314.319	3181.911	-33.919
5000	868.962	2411.837	1672.956	3694.404	309.240	3240.571	-33.853

3.136. Picene



Other names: 1,2:7,8-Dibenzphenanthrene

Formula: C₂₂H₁₄

Mass: 278.347 g/mol

CAS Number: 213-46-7

Point Group: C_{2v}

Length: 15.91 Å

Width: 7.962 Å

Breadth: 3.883 Å

L/B Ratio: 1.998

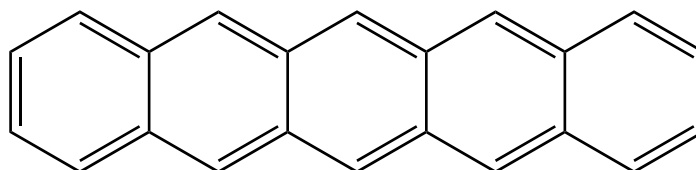
Cartesian coordinates:

C	4.9688	-1.6321	0.0000	C	-1.4107	-0.4487	0.0000	H	5.4905	1.7380	0.0000
C	5.6581	-0.4055	0.0000	C	-0.7171	0.7671	0.0000	H	3.0441	-2.6074	0.0000
C	4.9607	0.7786	0.0000	C	-1.4563	1.9951	0.0000	H	3.3698	2.9455	0.0000
C	3.5950	-1.6545	0.0000	C	-2.8126	2.0006	0.0000	H	0.8852	2.9379	0.0000
C	2.8542	-0.4498	0.0000	C	-2.8538	-0.4518	0.0000	H	-1.2485	-2.6127	0.0000
C	3.5469	0.7740	0.0000	C	-3.5475	0.7715	0.0000	H	1.2503	-2.6119	0.0000
C	2.8111	2.0026	0.0000	C	-4.9613	0.7750	0.0000	H	-0.8873	2.9373	0.0000
C	1.4549	1.9962	0.0000	C	-5.6578	-0.4097	0.0000	H	-3.3720	2.9431	0.0000
C	1.4110	-0.4478	0.0000	C	-4.9675	-1.6358	0.0000	H	-5.4919	1.7340	0.0000
C	0.7166	0.7676	0.0000	C	-3.5938	-1.6571	0.0000	H	-6.7527	-0.4091	0.0000
C	-0.6811	-1.6693	0.0000	H	5.5368	-2.5681	0.0000	H	-5.5348	-2.5722	0.0000
C	0.6822	-1.6688	0.0000	H	6.7530	-0.4041	0.0000	H	-3.0421	-2.6096	0.0000

Table 3.136: Table of thermodynamic data as a function of temperature for Picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-42.615	346.827	346.827	∞
100	94.842	326.565	691.562	-36.500	370.405	410.352	-214.342
200	182.243	417.470	531.902	-22.886	357.989	455.232	-118.892
250	233.992	463.646	513.612	-12.492	352.099	480.225	-100.335
298.15	284.785	509.210	509.210	0.000	346.827	505.392	-88.541
300	286.717	510.977	509.215	0.529	346.633	506.375	-88.166
350	337.614	559.034	512.894	16.149	341.748	533.396	-79.603
400	384.916	607.250	521.676	34.230	337.485	561.065	-73.266
450	427.826	655.109	533.849	54.567	333.780	589.238	-68.396
500	466.223	702.211	548.338	76.937	330.560	617.816	-64.541
600	530.723	793.146	581.628	126.911	325.315	675.786	-58.831
700	581.885	878.947	618.037	182.637	321.469	734.526	-54.810
800	623.070	959.431	655.736	242.956	318.855	793.717	-51.823
900	656.766	1034.827	693.714	307.002	317.313	853.166	-49.515
1000	684.708	1105.515	731.397	374.118	316.695	912.746	-47.676
1100	708.122	1171.905	768.456	443.793	316.829	972.358	-46.172
1200	727.902	1234.391	804.707	515.622	317.590	1031.914	-44.917
1300	744.727	1293.337	840.048	589.275	318.818	1091.397	-43.852
1400	759.123	1349.067	874.434	664.486	320.401	1150.774	-42.935
1500	771.508	1401.874	907.852	741.033	322.264	1210.030	-42.136
1600	782.217	1452.016	940.309	818.732	324.296	1269.147	-41.433
1700	791.521	1499.724	971.824	897.430	326.432	1328.113	-40.807
1800	799.643	1545.201	1002.425	976.997	328.607	1387.005	-40.249
1900	806.764	1588.630	1032.143	1057.325	330.793	1445.733	-39.745
2000	813.034	1630.175	1061.014	1138.321	332.941	1504.368	-39.289
2100	818.579	1669.980	1089.071	1219.908	334.988	1562.886	-38.874
2200	823.500	1708.176	1116.350	1302.016	336.929	1621.312	-38.494
2300	827.885	1744.880	1142.885	1384.590	338.760	1679.650	-38.145
2400	831.806	1780.199	1168.708	1467.578	340.421	1737.873	-37.823
2500	835.324	1814.228	1193.853	1550.938	341.920	1796.124	-37.527
2600	838.491	1847.052	1218.348	1634.631	343.228	1854.222	-37.251
2700	841.350	1878.752	1242.224	1718.625	344.346	1912.331	-36.996
2800	843.940	1909.397	1265.507	1802.892	345.254	1970.423	-36.758
2900	846.292	1939.054	1288.225	1887.405	345.925	2028.442	-36.535
3000	848.433	1967.781	1310.400	1972.143	346.396	2086.461	-36.328
3100	850.389	1995.634	1332.058	2057.086	346.603	2144.409	-36.132
3200	852.178	2022.661	1353.219	2142.216	346.578	2202.412	-35.950
3300	853.819	2048.909	1373.904	2227.517	346.308	2260.451	-35.779
3400	855.329	2074.421	1394.134	2312.975	345.768	2318.434	-35.618
3500	856.719	2099.235	1413.927	2398.578	344.962	2376.420	-35.465
3600	858.002	2123.388	1433.301	2484.315	343.908	2434.503	-35.323
3700	859.189	2146.913	1452.271	2570.176	342.581	2492.636	-35.189
3800	860.289	2169.841	1470.854	2656.150	340.956	2550.756	-35.062
3900	861.311	2192.201	1489.064	2742.231	339.070	2608.883	-34.941
4000	862.260	2214.019	1506.917	2828.410	336.907	2667.174	-34.829
4100	863.145	2235.322	1524.424	2914.681	334.439	2725.462	-34.722
4200	863.970	2256.131	1541.599	3001.037	331.688	2783.806	-34.621
4300	864.740	2276.470	1558.453	3087.473	328.642	2842.146	-34.525
4400	865.462	2296.358	1574.999	3173.983	325.309	2900.636	-34.434
4500	866.137	2315.815	1591.246	3260.564	321.701	2959.252	-34.349
4600	866.771	2334.859	1607.205	3347.209	317.774	3017.955	-34.269
4700	867.366	2353.507	1622.886	3433.917	313.541	3076.654	-34.192
4800	867.926	2371.774	1638.298	3520.681	309.041	3135.533	-34.121
4900	868.453	2389.675	1653.450	3607.501	304.213	3194.399	-34.052
5000	868.950	2407.225	1668.351	3694.371	299.132	3253.521	-33.989

3.137. Pentacene



Other names: Benzo[*b*]naphthacene
2,3:6,7-Dibenzanthracene
 β,β' -Dibenzanthracene
2,3,6,7-Dibenzoanthracene
lin-Dinaphthantracene
lin-Naphthanthrene

Formula: C₂₂H₁₄
Mass: 278.347 g/mol
CAS Number: 135-48-8
Point Group: D_{2h}

Length: 16.49 Å
Width: 7.424 Å
Breadth: 3.882 Å
L/B Ratio: 2.222

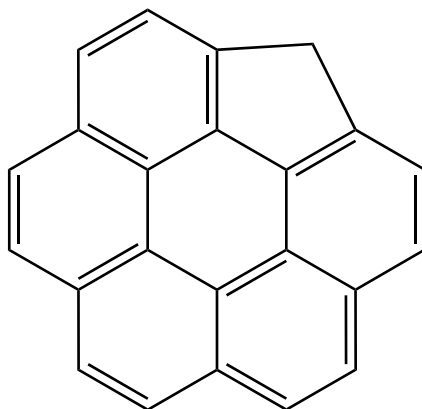
Cartesian coordinates:

C	6.0798	-0.7183	0.0000	C	-1.2161	-0.7138	0.0000	H	4.9061	2.5025	0.0000
C	6.0802	0.7156	0.0000	C	-1.2158	0.7143	0.0000	H	4.9050	-2.5047	0.0000
C	4.9162	1.4066	0.0000	C	-2.4561	1.4075	0.0000	H	2.4507	2.5035	0.0000
C	4.9156	-1.4087	0.0000	C	-2.4567	-1.4064	0.0000	H	2.4495	-2.5045	0.0000
C	3.6488	-0.7189	0.0000	C	-3.6491	-0.7173	0.0000	H	0.0004	2.5023	0.0000
C	3.6491	0.7174	0.0000	C	-3.6488	0.7189	0.0000	H	-0.0007	-2.5022	0.0000
C	2.4567	1.4064	0.0000	C	-4.9155	1.4087	0.0000	H	-2.4497	2.5045	0.0000
C	2.4561	-1.4075	0.0000	C	-6.0798	0.7182	0.0000	H	-2.4508	-2.5034	0.0000
C	1.2157	-0.7143	0.0000	C	-6.0801	-0.7156	0.0000	H	-4.9051	2.5046	0.0000
C	1.2160	0.7138	0.0000	C	-4.9161	-1.4066	0.0000	H	-7.0435	1.2378	0.0000
C	0.0004	1.4051	0.0000	H	7.0436	-1.2379	0.0000	H	-7.0440	-1.2348	0.0000
C	-0.0003	-1.4051	0.0000	H	7.0441	1.2347	0.0000	H	-4.9061	-2.5025	0.0000

Table 3.137: Table of thermodynamic data as a function of temperature for Pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-42.493	411.236	411.236	∞
100	93.253	317.188	682.747	-36.556	434.758	475.642	-248.445
200	182.733	407.684	522.632	-22.990	422.294	521.495	-136.198
250	235.106	454.043	504.256	-12.553	416.446	546.973	-114.281
298.15	286.182	499.831	499.831	0.000	411.236	572.597	-100.315
300	288.121	501.607	499.837	0.531	411.044	573.597	-99.870
350	339.063	549.886	503.533	16.224	406.231	601.081	-89.705
400	386.285	598.292	512.354	34.375	402.040	629.202	-82.164
450	429.068	646.304	524.576	54.778	398.399	657.820	-76.356
500	467.337	693.531	539.118	77.206	395.238	686.834	-71.752
600	531.636	784.650	572.514	127.281	390.094	745.663	-64.914
700	582.680	870.582	609.021	183.092	386.333	805.245	-60.087
800	623.801	951.167	646.808	243.487	383.795	865.268	-56.495
900	657.459	1026.647	684.865	307.605	382.324	925.539	-53.716
1000	685.373	1097.407	722.618	374.788	381.774	985.933	-51.499
1100	708.761	1163.859	759.742	444.529	381.973	1046.353	-49.686
1200	728.515	1226.400	796.050	516.420	382.796	1106.711	-48.173
1300	745.311	1285.393	831.444	590.133	384.085	1166.990	-46.889
1400	759.677	1341.166	865.879	665.401	385.725	1227.160	-45.785
1500	772.031	1394.010	899.342	742.002	387.641	1287.203	-44.823
1600	782.710	1444.185	931.840	819.751	389.724	1347.105	-43.978
1700	791.984	1491.921	963.393	898.497	391.907	1406.853	-43.226
1800	800.078	1537.424	994.030	978.109	394.128	1466.525	-42.557
1900	807.173	1580.876	1023.782	1058.479	396.356	1526.029	-41.953
2000	813.418	1622.441	1052.683	1139.515	398.544	1585.438	-41.407
2100	818.939	1662.264	1080.769	1221.139	400.627	1644.728	-40.910
2200	823.838	1700.476	1108.075	1303.282	402.604	1703.925	-40.455
2300	828.203	1737.195	1134.635	1385.889	404.467	1763.032	-40.039
2400	832.105	1772.527	1160.483	1468.907	406.159	1822.024	-39.654
2500	835.605	1806.568	1185.649	1552.296	407.688	1881.041	-39.301
2600	838.756	1839.403	1210.166	1636.017	409.022	1939.904	-38.972
2700	841.600	1871.112	1234.062	1720.037	410.167	1998.778	-38.668
2800	844.176	1901.767	1257.364	1804.328	411.098	2057.634	-38.385
2900	846.515	1931.431	1280.099	1888.864	411.793	2116.414	-38.120
3000	848.644	1960.166	1302.291	1973.624	412.285	2175.196	-37.873
3100	850.588	1988.025	1323.965	2058.587	412.512	2233.905	-37.640
3200	852.367	2015.059	1345.141	2143.736	412.508	2292.669	-37.423
3300	853.999	2041.313	1365.841	2229.056	412.255	2351.468	-37.220
3400	855.499	2066.830	1386.085	2314.531	411.733	2410.210	-37.028
3500	856.881	2091.649	1405.891	2400.151	410.944	2468.955	-36.846
3600	858.157	2115.806	1425.277	2485.904	409.906	2527.796	-36.677
3700	859.337	2139.335	1444.259	2571.780	408.593	2586.687	-36.517
3800	860.430	2162.267	1462.854	2657.769	406.983	2645.565	-36.365
3900	861.445	2184.630	1481.075	2743.863	405.111	2704.449	-36.221
4000	862.389	2206.452	1498.938	2830.055	402.961	2763.497	-36.087
4100	863.267	2227.758	1516.455	2916.339	400.505	2822.541	-35.959
4200	864.087	2248.570	1533.640	3002.707	397.766	2881.642	-35.838
4300	864.853	2268.912	1550.504	3089.154	394.732	2940.738	-35.722
4400	865.570	2288.802	1567.058	3175.676	391.410	2999.984	-35.614
4500	866.241	2308.262	1583.314	3262.267	387.812	3059.355	-35.511
4600	866.871	2327.308	1599.281	3348.923	383.896	3118.813	-35.415
4700	867.462	2345.957	1614.970	3435.640	379.673	3178.268	-35.322
4800	868.018	2364.226	1630.390	3522.414	375.182	3237.901	-35.235
4900	868.542	2382.130	1645.550	3609.242	370.363	3297.522	-35.151
5000	869.036	2399.682	1660.457	3696.121	365.291	3357.398	-35.074

3.138. 1*H*-Benzo[*ghi*]cyclopenta[*pqr*]perylene



Formula: C₂₃H₁₂
Mass: 288.341 g/mol
CAS Number: 64503-02-2
Point Group: C_{2v}

Length: 11.85 Å
Width: 11.24 Å
Breadth: 4.181 Å
L/B Ratio: 1.054

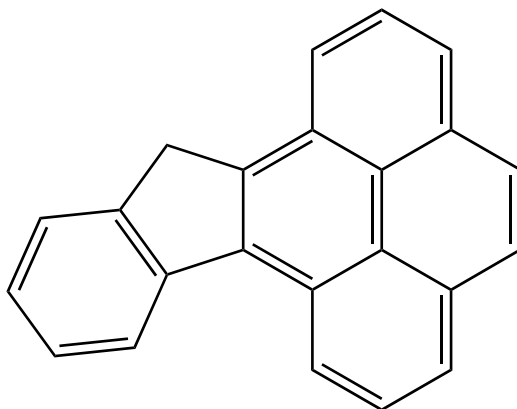
Cartesian coordinates:

C	-0.6032	3.4797	-0.0012	C	-0.0759	-3.5957	0.0008	H	-0.7150	4.1238	0.8880
C	0.4798	1.3963	-0.0077	C	-0.5111	-1.2285	-0.0055	H	2.4274	4.1376	0.0103
C	0.7498	2.7587	-0.0018	C	-1.0150	-2.5296	-0.0016	H	4.1345	2.3565	0.0107
C	2.1114	3.0898	0.0047	C	-2.4476	-2.6886	0.0014	H	4.7410	-0.2115	0.0067
C	3.0751	2.0751	0.0053	C	-3.3102	-1.6298	0.0028	H	3.9226	-2.5409	0.0045
C	1.3967	0.3548	-0.0059	C	-1.4346	-0.1360	-0.0056	H	1.9832	-4.2023	0.0034
C	2.7565	0.6946	0.0006	C	-2.8295	-0.2735	0.0006	H	-0.4533	-4.6246	0.0028
C	3.6656	-0.4208	0.0035	C	-3.5941	0.9192	0.0062	H	-2.8387	-3.7127	0.0031
C	3.2097	-1.7081	0.0024	C	-3.0280	2.1991	0.0071	H	-4.3933	-1.7946	0.0059
C	0.8947	-0.9848	-0.0054	C	-1.6344	2.3450	0.0003	H	-4.6864	0.8277	0.0115
C	1.8071	-2.0405	-0.0011	C	-0.9215	1.1532	-0.0069	H	-3.6780	3.0795	0.0145
C	1.2815	-3.3604	0.0011	H	-0.7141	4.1200	-0.8934				

Table 3.138: Table of thermodynamic data as a function of temperature for 1*H*-Benzo[*ghi*]cyclopenta[*pqr*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-39.260	372.703	372.703	∞
100	79.202	304.636	646.833	-34.220	394.084	426.246	-222.644
200	171.450	386.222	495.827	-21.921	382.721	462.948	-120.907
250	224.287	430.126	478.263	-12.034	377.424	483.618	-101.044
298.15	275.421	474.016	474.016	0.000	372.703	504.510	-88.386
300	277.358	475.725	474.021	0.511	372.528	505.327	-87.983
350	328.280	522.344	477.587	15.665	368.155	527.815	-78.770
400	375.511	569.309	486.116	33.277	364.329	550.884	-71.937
450	418.336	616.055	497.961	53.142	360.984	574.408	-66.674
500	456.652	662.153	512.082	75.036	358.052	598.299	-62.503
600	520.941	751.326	544.588	124.043	353.191	646.828	-56.310
700	571.741	835.595	580.203	178.775	349.516	696.079	-51.941
800	612.375	914.690	617.124	238.053	346.893	745.770	-48.693
900	645.362	988.787	654.348	300.995	345.186	795.728	-46.182
1000	672.495	1058.232	691.301	366.931	344.269	845.844	-44.181
1100	695.054	1123.418	727.652	435.342	343.984	896.028	-42.548
1200	713.978	1184.731	763.213	505.821	344.222	946.199	-41.186
1300	729.973	1242.529	797.882	578.041	344.839	996.343	-40.033
1400	743.584	1297.137	831.611	651.736	345.730	1046.432	-39.042
1500	755.237	1348.846	864.385	726.692	346.836	1096.451	-38.181
1600	765.272	1397.917	896.210	802.730	348.053	1146.385	-37.425
1700	773.959	1444.578	927.106	879.702	349.325	1196.221	-36.755
1800	781.519	1489.035	957.099	957.484	350.592	1246.035	-36.158
1900	788.129	1531.471	986.221	1035.974	351.833	1295.735	-35.621
2000	793.937	1572.047	1014.505	1115.083	353.005	1345.393	-35.137
2100	799.061	1610.910	1041.987	1194.738	354.047	1394.984	-34.698
2200	803.601	1648.189	1068.700	1274.876	354.960	1444.529	-34.297
2300	807.639	1684.001	1094.679	1355.442	355.741	1494.037	-33.930
2400	811.245	1718.452	1119.956	1436.389	356.332	1543.474	-33.592
2500	814.477	1751.635	1144.564	1517.678	356.746	1592.983	-33.283
2600	817.382	1783.637	1168.532	1599.274	356.954	1642.383	-32.995
2700	820.003	1814.535	1191.889	1681.145	356.959	1691.841	-32.730
2800	822.374	1844.400	1214.663	1763.266	356.742	1741.318	-32.484
2900	824.526	1873.297	1236.879	1845.613	356.279	1790.764	-32.254
3000	826.484	1901.283	1258.561	1928.165	355.607	1840.253	-32.041
3100	828.270	1928.413	1279.734	2010.904	354.662	1889.702	-31.841
3200	829.904	1954.736	1300.419	2093.814	353.480	1939.248	-31.654
3300	831.402	1980.296	1320.636	2176.880	352.046	1988.868	-31.481
3400	832.778	2005.137	1340.404	2260.090	350.337	2038.461	-31.316
3500	834.046	2029.296	1359.744	2343.432	348.358	2088.094	-31.162
3600	835.215	2052.808	1378.670	2426.896	346.128	2137.862	-31.019
3700	836.296	2075.707	1397.201	2510.472	343.620	2187.708	-30.884
3800	837.298	2098.023	1415.351	2594.153	340.815	2237.577	-30.757
3900	838.228	2119.784	1433.136	2677.929	337.744	2287.478	-30.637
4000	839.092	2141.018	1450.569	2761.796	334.397	2337.579	-30.525
4100	839.896	2161.747	1467.663	2845.746	330.743	2387.705	-30.419
4200	840.646	2181.995	1484.430	2929.773	326.805	2437.917	-30.319
4300	841.347	2201.785	1500.884	3013.873	322.573	2488.150	-30.224
4400	842.002	2221.134	1517.034	3098.041	318.054	2538.561	-30.136
4500	842.616	2240.063	1532.892	3182.273	313.261	2589.124	-30.053
4600	843.192	2258.590	1548.467	3266.563	308.148	2639.807	-29.975
4700	843.733	2276.729	1563.770	3350.910	302.731	2690.508	-29.901
4800	844.241	2294.498	1578.809	3435.309	297.046	2741.416	-29.832
4900	844.720	2311.911	1593.593	3519.757	291.032	2792.331	-29.766
5000	845.171	2328.981	1608.131	3604.252	284.768	2843.528	-29.706

3.139. 9H-Indeno[1,2-e]pyrene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-65-4
Point Group: C_s

Length: 13.41 Å
Width: 10.45 Å
Breadth: 4.178 Å
L/B Ratio: 1.284

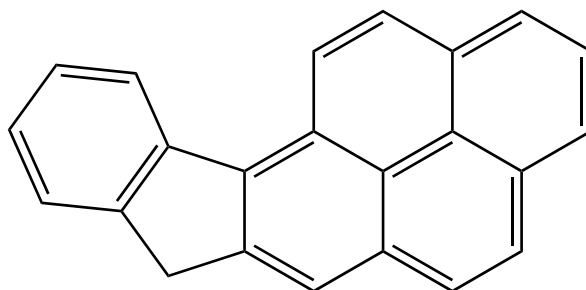
Cartesian coordinates:

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C	3.0680	0.7034	0.0000	C	-0.7642	3.0350	0.0000	H	6.2767	-0.3594	0.0000
C	2.4042	-0.5487	0.0000	C	-2.0565	3.5433	-0.0000	H	4.9517	1.7564	0.0000
C	3.1469	-1.7203	-0.0000	C	-3.1527	2.6893	-0.0000	H	-3.2793	-3.5551	0.0000
C	4.5391	-1.6344	-0.0000	C	-1.4597	-0.6512	0.0000	H	-0.9906	-4.5150	0.0000
C	5.1826	-0.4016	0.0000	C	-1.6583	0.7706	0.0000	H	0.9925	-3.0457	0.0000
C	4.4480	0.7850	0.0000	C	-2.9683	1.3035	0.0000	H	0.0963	3.7139	0.0000
C	0.9582	-0.2946	0.0000	C	-4.0928	0.4030	0.0000	H	-2.2129	4.6272	-0.0000
C	0.7565	1.0697	0.0000	C	-3.9096	-0.9359	0.0000	H	-4.1684	3.1008	-0.0000
C	-0.1533	-1.2084	0.0000	C	-2.5863	-1.5069	0.0000	H	-5.0994	0.8367	0.0000
C	-2.4060	-2.8930	0.0000	H	2.1642	2.4644	0.8893	H	-4.7643	-1.6224	0.0000
C	-1.1253	-3.4281	0.0000	H	2.1642	2.4644	-0.8893				
C	-0.0110	-2.5987	0.0000	H	2.6547	-2.7015	-0.0000				

Table 3.139: Table of thermodynamic data as a function of temperature for 9*H*-Indeno[1,2-*e*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-43.120	349.658	349.658	∞
100	94.065	332.072	703.266	-37.119	373.608	413.099	-215.776
200	185.540	423.815	540.624	-23.362	361.009	457.600	-119.510
250	238.855	470.895	521.947	-12.763	355.028	482.440	-100.798
298.15	291.199	517.447	517.447	0.000	349.658	507.479	-88.906
300	293.192	519.255	517.453	0.541	349.460	508.457	-88.528
350	345.757	568.435	521.217	16.526	344.469	535.362	-79.897
400	394.718	617.847	530.208	35.056	340.104	562.929	-73.510
450	439.210	666.952	542.679	55.923	336.300	591.015	-68.602
500	479.073	715.331	557.532	78.899	332.988	619.515	-64.719
600	546.094	808.840	591.691	130.289	327.581	677.356	-58.968
700	599.248	897.166	629.086	187.656	323.603	735.990	-54.919
800	641.977	980.074	667.834	249.792	320.885	795.093	-51.913
900	676.862	1057.769	706.890	315.791	319.261	854.465	-49.591
1000	705.720	1130.624	745.659	384.964	318.577	913.977	-47.740
1100	729.842	1199.051	783.799	456.777	318.655	973.526	-46.228
1200	750.175	1263.452	821.113	530.807	319.366	1033.025	-44.965
1300	767.434	1324.198	857.498	606.710	320.545	1092.454	-43.894
1400	782.175	1381.624	892.903	684.210	322.077	1151.782	-42.973
1500	794.835	1436.031	927.314	763.076	323.885	1210.992	-42.170
1600	805.767	1487.686	960.737	843.119	325.856	1270.067	-41.463
1700	815.253	1536.827	993.191	924.181	327.924	1328.995	-40.834
1800	823.525	1583.665	1024.704	1006.129	330.023	1387.855	-40.274
1900	830.771	1628.389	1055.309	1088.852	332.125	1446.553	-39.768
2000	837.146	1671.168	1085.040	1172.254	334.180	1505.163	-39.310
2100	842.779	1712.151	1113.934	1256.256	336.123	1563.661	-38.893
2200	847.776	1751.475	1142.025	1340.789	337.952	1622.073	-38.512
2300	852.226	1789.260	1169.350	1425.793	339.660	1680.402	-38.162
2400	856.202	1825.616	1195.942	1511.219	341.189	1738.620	-37.839
2500	859.769	1860.642	1221.833	1597.020	342.545	1796.874	-37.543
2600	862.978	1894.426	1247.056	1683.160	343.699	1854.978	-37.266
2700	865.875	1927.050	1271.641	1769.606	344.655	1913.103	-37.010
2800	868.497	1958.588	1295.615	1856.326	345.388	1971.216	-36.773
2900	870.878	1989.107	1319.005	1943.297	345.875	2029.261	-36.550
3000	873.046	2018.668	1341.837	2030.495	346.152	2087.315	-36.343
3100	875.024	2047.328	1364.135	2117.900	346.153	2145.300	-36.147
3200	876.835	2075.138	1385.921	2205.494	345.913	2203.350	-35.965
3300	878.495	2102.145	1407.218	2293.262	345.417	2261.445	-35.795
3400	880.021	2128.394	1428.044	2381.189	344.641	2319.486	-35.634
3500	881.427	2153.924	1448.421	2469.262	343.588	2377.538	-35.482
3600	882.724	2178.773	1468.365	2557.470	342.277	2435.698	-35.340
3700	883.924	2202.976	1487.894	2645.804	340.683	2493.914	-35.207
3800	885.036	2226.563	1507.023	2734.252	338.780	2552.124	-35.081
3900	886.068	2249.566	1525.769	2822.808	336.606	2610.345	-34.961
4000	887.027	2272.012	1544.146	2911.463	334.145	2668.743	-34.849
4100	887.921	2293.926	1562.167	3000.211	331.368	2727.143	-34.744
4200	888.754	2315.333	1579.845	3089.046	328.299	2785.607	-34.643
4300	889.533	2336.255	1597.194	3177.960	324.923	2844.072	-34.548
4400	890.261	2356.713	1614.224	3266.950	321.252	2902.697	-34.459
4500	890.944	2376.727	1630.947	3356.011	317.294	2961.457	-34.375
4600	891.584	2396.316	1647.373	3445.138	313.008	3020.313	-34.296
4700	892.185	2415.497	1663.513	3534.327	308.405	3079.170	-34.220
4800	892.750	2434.287	1679.376	3623.574	303.525	3138.217	-34.150
4900	893.282	2452.700	1694.971	3712.875	298.304	3197.255	-34.082
5000	893.784	2470.752	1710.306	3802.229	292.824	3256.563	-34.020

3.140. 7H-Indeno[1,2-a]pyrene



Formula: $C_{23}H_{14}$
Mass: 290.357 g/mol
CAS Number: 87308-64-3
Point Group: C_s

Length: 14.81 Å
Width: 9.590 Å
Breadth: 4.176 Å
L/B Ratio: 1.544

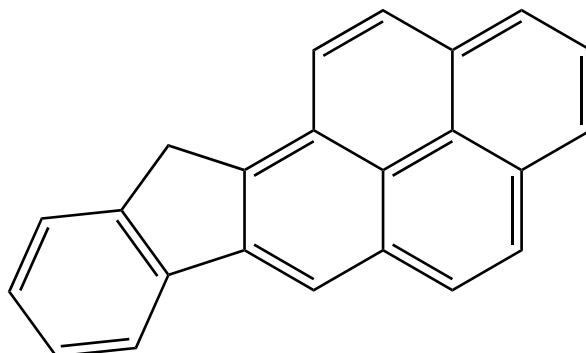
Cartesian coordinates:

C	4.5632	-1.8785	-0.0000	C	-3.5258	0.6129	0.0000	H	2.4952	-2.5249	-0.0000
C	5.4498	-0.8084	0.0000	C	-4.7933	0.0199	0.0000	H	3.1171	2.6324	0.8886
C	4.9792	0.5063	0.0000	C	-4.9197	-1.3626	0.0000	H	3.1171	2.6324	-0.8886
C	3.1833	-1.6695	-0.0000	C	-3.7927	-2.1772	0.0000	H	0.4198	3.4871	0.0000
C	2.7028	-0.3687	-0.0000	C	0.0867	-0.4446	-0.0000	H	-2.0183	3.6957	-0.0000
C	3.6132	0.7170	0.0000	C	-1.0664	0.3882	-0.0000	H	-4.2735	2.6621	-0.0000
C	2.8735	2.0211	0.0000	C	-2.3730	-0.2048	0.0000	H	-5.6873	0.6538	0.0000
C	1.3392	0.1709	-0.0000	C	-2.5157	-1.6114	0.0000	H	-5.9162	-1.8167	0.0000
C	1.4361	1.5856	0.0000	C	-1.3303	-2.4294	0.0000	H	-3.9036	-3.2675	0.0000
C	0.3209	2.3961	0.0000	C	-0.0986	-1.8736	0.0000	H	-1.4573	-3.5182	0.0000
C	-0.9482	1.7965	-0.0000	H	4.9504	-2.9028	-0.0000	H	0.7968	-2.5105	0.0000
C	-2.1386	2.6062	-0.0000	H	6.5287	-0.9953	0.0000				
C	-3.3687	2.0435	-0.0000	H	5.6756	1.3504	0.0000				

Table 3.140: Table of thermodynamic data as a function of temperature for 7*H*-Indeno[1,2-*a*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-43.340	345.914	345.914	∞
100	94.440	335.254	707.806	-37.255	369.727	408.900	-213.583
200	186.219	427.266	544.550	-23.457	357.170	453.070	-118.327
250	239.850	474.534	525.797	-12.816	351.231	477.733	-99.815
298.15	292.378	521.279	521.279	0.000	345.914	502.592	-88.050
300	294.376	523.093	521.284	0.543	345.717	503.563	-87.676
350	347.017	572.463	525.063	16.590	340.788	530.271	-79.137
400	395.976	622.044	534.088	35.183	336.486	557.633	-72.818
450	440.423	671.295	546.602	56.112	332.745	585.505	-67.962
500	480.218	719.798	561.504	79.147	329.492	613.785	-64.120
600	547.087	813.503	595.763	130.644	324.191	671.169	-58.429
700	600.101	901.972	633.253	188.103	320.306	729.329	-54.422
800	642.713	984.985	672.087	250.318	317.667	787.946	-51.447
900	677.502	1062.761	711.221	316.386	316.111	846.822	-49.147
1000	706.281	1135.679	750.060	385.619	315.488	905.831	-47.315
1100	730.339	1204.157	788.261	457.485	315.619	964.873	-45.817
1200	750.617	1268.598	825.631	531.561	316.376	1023.859	-44.567
1300	767.830	1329.378	862.065	607.506	317.597	1082.772	-43.505
1400	782.530	1386.832	897.515	685.043	319.166	1141.580	-42.592
1500	795.156	1441.263	931.967	763.943	321.008	1200.268	-41.796
1600	806.058	1492.937	965.426	844.017	323.010	1258.819	-41.095
1700	815.518	1542.095	997.914	925.107	325.105	1317.221	-40.472
1800	823.767	1588.947	1029.458	1007.080	327.230	1375.553	-39.917
1900	830.993	1633.684	1060.091	1089.826	329.355	1433.723	-39.415
2000	837.350	1676.473	1089.848	1173.250	331.432	1491.803	-38.961
2100	842.967	1717.466	1118.766	1257.272	333.394	1549.770	-38.548
2200	847.950	1756.799	1146.879	1341.823	335.241	1607.649	-38.170
2300	852.387	1794.591	1174.224	1426.844	336.966	1665.446	-37.823
2400	856.352	1830.954	1200.835	1512.284	338.510	1723.130	-37.502
2500	859.908	1865.985	1226.745	1598.100	339.881	1780.850	-37.208
2600	863.108	1899.775	1251.985	1684.254	341.049	1838.420	-36.934
2700	865.997	1932.404	1276.585	1770.712	342.016	1896.010	-36.680
2800	868.611	1963.946	1300.573	1857.444	342.762	1953.587	-36.444
2900	870.985	1994.469	1323.977	1944.426	343.259	2011.096	-36.223
3000	873.147	2024.034	1346.822	2031.634	343.547	2068.614	-36.017
3100	875.119	2052.697	1369.133	2119.049	343.558	2126.062	-35.823
3200	876.924	2080.510	1390.931	2206.652	343.327	2183.575	-35.642
3300	878.579	2107.520	1412.238	2294.429	342.839	2241.133	-35.473
3400	880.101	2133.771	1433.075	2382.364	342.071	2298.636	-35.314
3500	881.502	2159.303	1453.462	2470.445	341.027	2356.151	-35.163
3600	882.796	2184.154	1473.415	2558.661	339.723	2413.772	-35.022
3700	883.992	2208.358	1492.953	2647.001	338.136	2471.450	-34.890
3800	885.101	2231.948	1512.091	2735.456	336.240	2529.121	-34.764
3900	886.130	2254.952	1530.845	2824.019	334.072	2586.804	-34.646
4000	887.086	2277.399	1549.229	2912.680	331.617	2644.664	-34.535
4100	887.977	2299.315	1567.258	3001.434	328.846	2702.525	-34.430
4200	888.808	2320.723	1584.944	3090.273	325.782	2760.450	-34.331
4300	889.584	2341.646	1602.299	3179.193	322.412	2818.375	-34.236
4400	890.310	2362.106	1619.336	3268.188	318.745	2876.461	-34.147
4500	890.991	2382.121	1636.065	3357.254	314.792	2934.682	-34.064
4600	891.629	2401.711	1652.497	3446.385	310.511	2992.999	-33.986
4700	892.228	2420.894	1668.643	3535.578	305.912	3051.316	-33.911
4800	892.792	2439.684	1684.511	3624.830	301.036	3109.824	-33.841
4900	893.322	2458.098	1700.111	3714.136	295.820	3168.322	-33.774
5000	893.822	2476.151	1715.452	3803.493	290.344	3227.090	-33.712

3.141. 1*H*-Indeno[2,1-*a*]pyrene



Other names: Indeno-2',3'-3,4-pyrene

Formula: C₂₃H₁₄

Mass: 290.357 g/mol

CAS Number: 196-36-1

Point Group: C_s

Length: 15.50 Å

Width: 9.207 Å

Breadth: 4.176 Å

L/B Ratio: 1.684

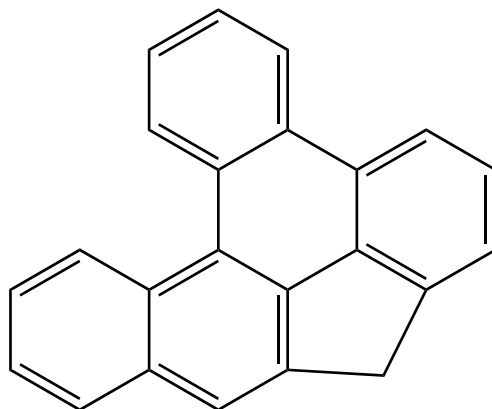
Cartesian coordinates:

C	1.6264	0.6122	0.0000	C	-2.5244	-0.0905	0.0000	H	-1.1429	3.5766	-0.0000
C	1.1416	-0.7175	0.0000	C	-3.0308	-1.4111	0.0000	H	-3.5906	3.1784	-0.0000
C	2.2896	-1.6892	-0.0000	C	-2.1043	-2.5163	0.0000	H	-5.4915	1.6149	-0.0000
C	0.7705	1.6979	0.0000	C	-0.7693	-2.3070	0.0000	H	-6.3641	-0.7075	0.0000
C	-0.6132	1.4617	0.0000	C	3.0878	0.5678	0.0000	H	-4.8088	-2.6389	0.0000
C	-1.5475	2.5579	-0.0000	C	3.4919	-0.7882	-0.0000	H	-2.5169	-3.5317	0.0000
C	-2.8830	2.3414	-0.0000	C	4.8329	-1.1227	-0.0000	H	-0.0626	-3.1451	0.0000
C	-3.4174	1.0044	-0.0000	C	5.7745	-0.0900	0.0000	H	5.1508	-2.1697	-0.0000
C	-4.7966	0.7676	-0.0000	C	5.3768	1.2422	0.0000	H	6.8414	-0.3368	0.0000
C	-5.2829	-0.5328	0.0000	C	4.0238	1.5878	0.0000	H	6.1336	2.0336	0.0000
C	-4.4120	-1.6174	0.0000	H	2.2693	-2.3475	0.8886	H	3.7089	2.6363	0.0000
C	-0.2241	-0.9730	0.0000	H	2.2693	-2.3475	-0.8886				
C	-1.1092	0.1377	0.0000	H	1.1633	2.7209	0.0000				

Table 3.141: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[2,1-*a*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-43.028	337.674	337.674	∞
100	93.574	328.594	699.923	-37.133	361.610	401.449	-209.691
200	185.619	420.127	537.138	-23.402	348.985	446.314	-116.563
250	239.295	467.266	518.426	-12.790	343.017	471.336	-98.478
298.15	291.867	513.916	513.916	0.000	337.674	496.548	-86.991
300	293.867	515.728	513.922	0.542	337.477	497.532	-86.626
350	346.548	565.022	517.695	16.565	332.524	524.610	-78.292
400	395.545	614.543	526.706	35.135	328.199	552.346	-72.128
450	440.028	663.746	539.204	56.043	324.437	580.594	-67.392
500	479.863	712.209	554.089	79.060	321.165	609.253	-63.647
600	546.817	805.856	588.314	130.525	315.833	667.399	-58.101
700	599.918	894.290	625.773	187.962	311.925	726.326	-54.198
800	642.609	977.284	664.581	250.163	309.272	785.712	-51.301
900	677.464	1055.052	703.693	316.223	307.709	845.359	-49.062
1000	706.295	1127.969	742.513	385.455	307.085	905.139	-47.279
1100	730.391	1196.449	780.699	457.325	307.219	964.952	-45.821
1200	750.696	1260.897	818.057	531.407	307.983	1024.708	-44.603
1300	767.927	1321.683	854.482	607.362	309.213	1084.391	-43.570
1400	782.638	1379.145	889.925	684.909	310.792	1143.968	-42.681
1500	795.270	1433.583	924.370	763.820	312.645	1203.424	-41.906
1600	806.175	1485.266	957.825	843.905	314.659	1262.743	-41.223
1700	815.635	1534.430	990.308	925.007	316.766	1321.911	-40.617
1800	823.883	1581.289	1021.849	1006.992	318.902	1381.010	-40.075
1900	831.106	1626.032	1052.480	1089.749	321.039	1439.945	-39.586
2000	837.460	1668.827	1082.235	1173.184	323.127	1498.790	-39.144
2100	843.072	1709.826	1111.151	1257.217	325.100	1557.521	-38.740
2200	848.051	1749.163	1139.264	1341.778	326.957	1616.165	-38.372
2300	852.483	1786.960	1166.608	1426.809	328.692	1674.724	-38.033
2400	856.444	1823.326	1193.218	1512.259	330.245	1733.172	-37.721
2500	859.996	1858.361	1219.128	1598.084	331.625	1791.654	-37.434
2600	863.192	1892.154	1244.367	1684.246	332.801	1849.986	-37.166
2700	866.076	1924.786	1268.967	1770.712	333.777	1908.338	-36.918
2800	868.687	1956.332	1292.956	1857.452	334.530	1966.677	-36.688
2900	871.058	1986.857	1316.360	1944.441	335.036	2024.947	-36.472
3000	873.216	2016.424	1339.205	2031.657	335.330	2083.226	-36.271
3100	875.185	2045.089	1361.516	2119.078	335.348	2141.435	-36.082
3200	876.987	2072.904	1383.314	2206.688	335.123	2199.709	-35.906
3300	878.639	2099.916	1404.622	2294.471	334.642	2258.027	-35.741
3400	880.158	2126.169	1425.460	2382.412	333.880	2316.291	-35.585
3500	881.557	2151.703	1445.846	2470.498	332.841	2374.565	-35.438
3600	882.848	2176.556	1465.800	2558.719	331.543	2432.947	-35.300
3700	884.042	2200.761	1485.338	2647.065	329.960	2491.384	-35.171
3800	885.149	2224.352	1504.477	2735.525	328.069	2549.815	-35.049
3900	886.175	2247.358	1523.232	2824.092	325.906	2608.258	-34.933
4000	887.130	2269.806	1541.616	2912.758	323.456	2666.877	-34.825
4100	888.019	2291.722	1559.645	3001.516	320.689	2725.497	-34.723
4200	888.848	2313.132	1577.332	3090.360	317.629	2784.181	-34.626
4300	889.623	2334.056	1594.688	3179.284	314.263	2842.866	-34.533
4400	890.348	2354.516	1611.725	3268.282	310.600	2901.710	-34.447
4500	891.026	2374.533	1628.454	3357.352	306.651	2960.690	-34.366
4600	891.663	2394.123	1644.887	3446.486	302.373	3019.766	-34.290
4700	892.261	2413.306	1661.033	3535.683	297.777	3078.842	-34.217
4800	892.824	2432.097	1676.902	3624.937	292.905	3138.108	-34.149
4900	893.353	2450.512	1692.503	3714.246	287.692	3197.365	-34.084
5000	893.852	2468.565	1707.844	3803.607	282.218	3256.892	-34.024

3.142. 8*H*-Benzo[*g*]cyclopenta[*mno*]chysene



Other names: 8*H*-Benzo[*p*]cyclopenta[*def*]chrysene

Formula: C₂₃H₁₄

Mass: 290.357 g/mol

CAS Number: 87308-57-4

Point Group: C₁

Length: 13.62 Å

Width: 11.18 Å

Breadth: 4.413 Å

L/B Ratio: 1.218

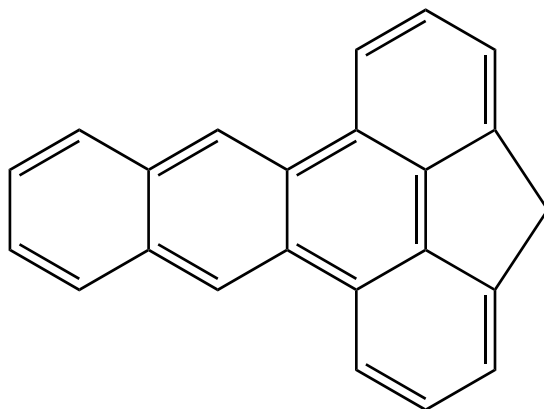
Cartesian coordinates:

C	-0.0624	0.8896	0.0543	C	-0.2249	-1.5022	0.0585	H	5.9511	0.3525	-0.0906
C	0.4776	2.2125	0.1297	C	-1.6416	-1.4009	-0.0545	H	4.4540	2.3039	0.2361
C	-0.6648	3.2096	0.1270	C	-2.4377	-2.5592	-0.0736	H	2.5506	-2.2240	-0.5132
C	-1.8988	2.3389	0.0226	C	-1.8736	-3.8095	0.0664	H	2.3199	3.3114	0.2867
C	-1.4832	0.9902	-0.0025	C	-0.4943	-3.9181	0.2616	H	-3.5251	-2.4361	-0.1894
C	4.3106	-1.0463	-0.3177	C	0.3030	-2.7905	0.2652	H	-2.4983	-4.7080	0.0442
C	4.8637	0.2269	-0.0953	C	-2.3094	-0.1114	-0.0967	H	-0.0457	-4.9049	0.4177
C	4.0330	1.3017	0.0925	C	-3.2501	2.5847	-0.0569	H	1.3750	-2.9186	0.4615
C	2.9497	-1.2250	-0.2972	C	-4.1276	1.4807	-0.1607	H	-3.6499	3.6028	-0.0436
C	2.0600	-0.1532	-0.0427	C	-3.6898	0.1670	-0.1818	H	-5.2026	1.6817	-0.2264
C	2.6243	1.1455	0.0934	H	-0.5878	3.9084	-0.7253	H	-4.3918	-0.6743	-0.2600
C	1.8264	2.3385	0.1909	H	-0.6742	3.8177	1.0494				
C	0.6217	-0.3039	0.0232	H	4.9756	-1.8938	-0.5143				

Table 3.142: Table of thermodynamic data as a function of temperature for 8*H*-Benzo[*g*]cyclopenta[*mno*]chysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.901	394.787	394.787	∞
100	93.392	325.813	696.600	-37.079	418.777	458.894	-239.697
200	185.348	417.305	534.079	-23.355	406.145	504.038	-131.638
250	238.781	464.354	515.405	-12.763	400.157	529.204	-110.569
298.15	291.268	510.905	510.905	0.000	394.787	554.558	-97.154
300	293.266	512.713	510.911	0.541	394.588	555.548	-96.727
350	345.961	561.915	514.676	16.534	389.605	582.779	-86.973
400	395.010	611.361	523.672	35.075	385.252	610.672	-79.744
450	439.548	660.504	536.150	55.959	381.465	639.081	-74.181
500	479.426	708.919	551.014	78.952	378.170	667.903	-69.774
600	546.421	802.491	585.196	130.377	372.797	726.382	-63.236
700	599.518	890.863	622.615	187.774	368.849	785.649	-58.625
800	642.187	973.803	661.386	249.934	366.155	845.380	-55.197
900	677.020	1051.520	700.463	315.951	364.550	905.378	-52.546
1000	705.837	1124.389	739.251	385.138	363.879	965.513	-50.432
1100	729.927	1192.826	777.407	456.961	363.968	1025.686	-48.705
1200	750.235	1257.233	814.735	530.997	364.685	1085.807	-47.263
1300	767.476	1317.983	851.132	606.906	365.870	1145.858	-46.040
1400	782.202	1375.412	886.549	684.409	367.405	1205.807	-44.988
1500	794.852	1429.821	920.969	763.277	369.215	1265.638	-44.073
1600	805.776	1481.476	954.400	843.322	371.187	1325.334	-43.267
1700	815.257	1530.617	986.862	924.384	373.256	1384.883	-42.551
1800	823.524	1577.455	1018.382	1006.333	375.355	1444.364	-41.913
1900	830.767	1622.179	1048.993	1089.055	377.457	1503.683	-41.338
2000	837.140	1664.958	1078.729	1172.457	379.512	1562.914	-40.818
2100	842.772	1705.941	1107.627	1256.459	381.454	1622.033	-40.345
2200	847.768	1745.264	1135.723	1340.990	383.282	1681.066	-39.913
2300	852.216	1783.049	1163.052	1425.994	384.989	1740.016	-39.516
2400	856.193	1819.405	1189.647	1511.418	386.517	1798.855	-39.150
2500	859.759	1854.430	1215.542	1597.219	387.872	1857.730	-38.814
2600	862.968	1888.214	1240.768	1683.358	389.025	1916.456	-38.501
2700	865.865	1920.838	1265.355	1769.802	389.980	1975.202	-38.212
2800	868.487	1952.375	1289.332	1856.522	390.712	2033.936	-37.943
2900	870.868	1982.894	1312.724	1943.491	391.198	2092.602	-37.691
3000	873.036	2012.455	1335.559	2030.688	391.474	2151.278	-37.456
3100	875.015	2041.114	1357.859	2118.092	391.474	2209.884	-37.236
3200	876.825	2068.924	1379.647	2205.686	391.233	2268.555	-37.030
3300	878.486	2095.931	1400.945	2293.452	390.736	2327.272	-36.837
3400	880.012	2122.179	1421.774	2381.378	389.959	2385.935	-36.655
3500	881.418	2147.709	1442.152	2469.451	388.905	2444.608	-36.483
3600	882.716	2172.558	1462.097	2557.658	387.594	2503.389	-36.322
3700	883.916	2196.760	1481.628	2645.991	385.998	2562.227	-36.171
3800	885.028	2220.348	1500.758	2734.439	384.095	2621.058	-36.028
3900	886.060	2243.350	1519.506	2822.994	381.920	2679.901	-35.893
4000	887.020	2265.795	1537.883	2911.648	379.459	2738.921	-35.766
4100	887.914	2287.709	1555.906	3000.396	376.681	2797.943	-35.645
4200	888.748	2309.116	1573.585	3089.229	373.611	2857.028	-35.532
4300	889.526	2330.038	1590.935	3178.143	370.235	2916.114	-35.423
4400	890.255	2350.496	1607.966	3267.133	366.562	2975.361	-35.321
4500	890.937	2370.511	1624.690	3356.193	362.604	3034.742	-35.226
4600	891.578	2390.099	1641.117	3445.319	358.317	3094.221	-35.135
4700	892.179	2409.280	1657.258	3534.507	353.714	3153.699	-35.049
4800	892.744	2428.070	1673.121	3623.753	348.833	3213.368	-34.968
4900	893.277	2446.483	1688.717	3713.055	343.612	3273.028	-34.890
5000	893.779	2464.535	1704.053	3802.408	338.131	3332.957	-34.818

3.143. 4*H*-Benzo[*b*]cyclopenta[*ijkl*]triphenylene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 143255-68-9
Point Group: C_{2v}

Length: 13.88 Å
Width: 10.94 Å
Breadth: 4.177 Å
L/B Ratio: 1.268

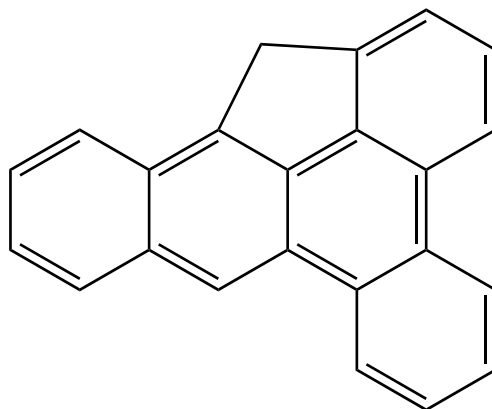
Cartesian coordinates:

C	-1.9098	0.7487	0.0000	C	0.4802	-0.7313	0.0000	H	6.3265	1.1245	-0.0000
C	-3.2240	1.2525	-0.0000	C	0.5063	0.7132	0.0000	H	4.2047	2.4218	-0.0000
C	-4.1841	0.0756	-0.0000	C	-0.7919	-1.4570	0.0000	H	4.1148	-2.5719	-0.0000
C	-3.2670	-1.1351	-0.0000	C	-3.4592	-2.5019	-0.0000	H	1.7436	2.4674	0.0000
C	-1.9356	-0.6793	0.0000	C	-2.3213	-3.3325	0.0000	H	1.6541	-2.5289	0.0000
C	5.3334	-0.8048	-0.0000	C	-1.0187	-2.8446	0.0000	H	-4.4614	-2.9399	-0.0000
C	5.3590	0.6120	-0.0000	C	-0.7387	1.4844	0.0000	H	-2.4747	-4.4174	0.0000
C	4.1938	1.3261	-0.0000	C	-0.9149	2.8794	0.0000	H	-0.1647	-3.5331	0.0000
C	4.1433	-1.4765	-0.0000	C	-2.1989	3.4142	0.0000	H	-0.0360	3.5359	0.0000
C	2.9138	-0.7584	0.0000	C	-3.3662	2.6253	-0.0000	H	-2.3128	4.5040	0.0000
C	2.9392	0.6526	0.0000	H	-4.8387	0.0876	-0.8895	H	-4.3519	3.0995	-0.0000
C	1.7204	1.3681	0.0000	H	-4.8387	0.0876	0.8895				
C	1.6699	-1.4295	0.0000	H	6.2819	-1.3519	-0.0000				

Table 3.143: Table of thermodynamic data as a function of temperature for 4*H*-Benzo[*b*]cyclopenta[*ijkl*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-43.005	377.878	377.878	∞
100	93.796	322.647	693.694	-37.105	401.843	442.276	-231.017
200	185.405	414.223	531.076	-23.371	389.221	487.730	-127.379
250	238.955	461.298	512.389	-12.773	383.239	513.050	-107.194
298.15	291.500	507.885	507.885	0.000	377.878	538.550	-94.350
300	293.500	509.695	507.891	0.541	377.680	539.546	-93.941
350	346.192	558.933	511.659	16.546	372.709	566.927	-84.607
400	395.208	608.407	520.661	35.098	368.367	594.968	-77.693
450	439.708	657.571	533.147	55.991	364.588	623.524	-72.375
500	479.554	706.002	548.019	78.991	361.301	652.493	-68.164
600	546.522	799.594	582.216	130.427	355.939	711.262	-61.920
700	599.629	887.983	619.648	187.834	352.002	770.817	-57.518
800	642.326	970.939	658.431	250.007	349.320	830.836	-54.247
900	677.189	1048.674	697.519	316.039	347.729	891.119	-51.718
1000	706.030	1121.562	736.318	385.244	347.078	951.539	-49.702
1100	730.138	1190.018	774.483	457.088	347.186	1011.993	-48.055
1200	750.456	1254.444	811.822	531.146	347.925	1072.394	-46.679
1300	767.700	1315.212	848.230	607.077	349.132	1132.723	-45.512
1400	782.426	1372.658	883.656	684.602	350.689	1192.948	-44.509
1500	795.072	1427.081	918.086	763.493	352.522	1253.054	-43.634
1600	805.990	1478.751	951.527	843.559	354.516	1313.023	-42.865
1700	815.462	1527.905	983.998	924.643	356.606	1372.844	-42.181
1800	823.721	1574.755	1015.526	1006.611	358.725	1432.595	-41.572
1900	830.955	1619.489	1046.145	1089.353	360.846	1492.184	-41.022
2000	837.319	1662.277	1075.890	1172.773	362.919	1551.684	-40.525
2100	842.941	1703.268	1104.796	1256.792	364.879	1611.071	-40.072
2200	847.928	1742.599	1132.899	1341.340	366.724	1670.370	-39.659
2300	852.369	1780.391	1160.235	1426.359	368.447	1729.586	-39.279
2400	856.337	1816.753	1186.837	1511.798	369.989	1788.691	-38.929
2500	859.896	1851.784	1212.739	1597.613	371.358	1847.831	-38.608
2600	863.097	1885.573	1237.971	1683.765	372.525	1906.821	-38.308
2700	865.987	1918.202	1262.564	1770.222	373.492	1965.831	-38.030
2800	868.604	1949.744	1286.546	1856.954	374.236	2024.828	-37.773
2900	870.979	1980.266	1309.944	1943.935	374.733	2083.757	-37.532
3000	873.141	2009.831	1332.783	2031.143	375.020	2142.695	-37.307
3100	875.114	2038.494	1355.088	2118.557	375.030	2201.564	-37.095
3200	876.920	2066.306	1376.881	2206.160	374.799	2260.497	-36.898
3300	878.576	2093.316	1398.184	2293.936	374.311	2319.475	-36.713
3400	880.098	2119.567	1419.017	2381.871	373.543	2378.399	-36.539
3500	881.500	2145.100	1439.399	2469.951	372.498	2437.334	-36.374
3600	882.794	2169.951	1459.349	2558.167	371.194	2496.376	-36.221
3700	883.991	2194.155	1478.883	2646.507	369.606	2555.474	-36.076
3800	885.099	2217.744	1498.017	2734.962	367.710	2614.566	-35.939
3900	886.128	2240.749	1516.768	2823.524	365.542	2673.669	-35.809
4000	887.085	2263.196	1535.149	2912.185	363.088	2732.949	-35.688
4100	887.976	2285.111	1553.175	3000.939	360.316	2792.231	-35.573
4200	888.807	2306.519	1570.858	3089.779	357.252	2851.576	-35.464
4300	889.584	2327.443	1588.210	3178.699	353.882	2910.922	-35.360
4400	890.310	2347.902	1605.244	3267.694	350.215	2970.428	-35.263
4500	890.990	2367.918	1621.971	3356.759	346.262	3030.069	-35.171
4600	891.628	2387.508	1638.401	3445.890	341.981	3089.806	-35.085
4700	892.228	2406.690	1654.544	3535.083	337.382	3149.544	-35.003
4800	892.791	2425.480	1670.410	3624.335	332.506	3209.472	-34.925
4900	893.322	2443.894	1686.008	3713.641	327.290	3269.390	-34.851
5000	893.822	2461.947	1701.347	3802.998	321.813	3329.579	-34.783

3.144. 1*H*-Benzo[*b*]cyclopenta[*def*]triphenylene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 197-79-5
Point Group: C_s

Length: 13.88 Å
Width: 10.85 Å
Breadth: 4.179 Å
L/B Ratio: 1.279

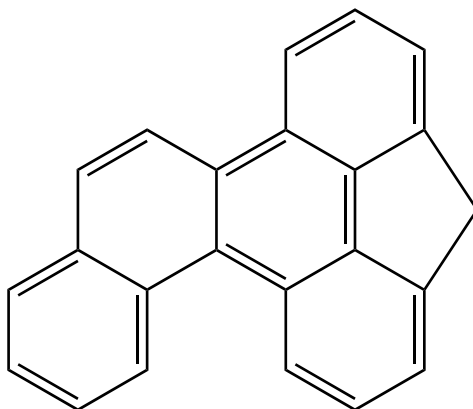
Cartesian coordinates:

C	-1.1872	3.6655	0.0105	C	-3.7822	-0.9007	-0.0073	H	5.7210	-2.1621	-0.0025
C	-0.2869	2.6192	0.0093	C	1.2272	2.5029	0.0119	H	3.4455	-3.1445	-0.0055
C	-0.8225	1.3174	0.0046	C	1.4658	1.0024	0.0050	H	4.0556	1.8119	0.0082
C	-2.1621	0.9719	0.0014	C	2.6158	0.1898	0.0025	H	1.0394	-2.9131	-0.0096
C	-3.0549	2.0576	0.0036	C	2.4251	-1.2231	-0.0019	H	-4.1355	1.8679	0.0018
C	-2.5619	3.3584	0.0075	C	1.1342	-1.8188	-0.0050	H	-3.2760	4.1895	0.0082
C	0.2372	0.3583	0.0020	C	3.5826	-2.0569	-0.0032	H	-0.8549	4.7077	0.0143
C	0.0015	-1.0239	-0.0028	C	4.8368	-1.5162	-0.0012	H	-0.9256	-3.5274	-0.0110
C	-1.4067	-1.4253	-0.0050	C	5.0165	-0.1103	0.0027	H	-3.3010	-4.2654	-0.0184
C	-2.4524	-0.4621	-0.0034	C	3.9347	0.7228	0.0047	H	-5.1294	-2.5801	-0.0145
C	-1.7366	-2.7863	-0.0099	H	1.6744	2.9878	-0.8743	H	-4.5858	-0.1518	-0.0058
C	-3.0596	-3.1975	-0.0137	H	1.6711	2.9786	0.9048				
C	-4.0846	-2.2527	-0.0123	H	6.0337	0.2948	0.0044				

Table 3.144: Table of thermodynamic data as a function of temperature for 1*H*-Benzo[*b*]cyclopenta[*def*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-43.112	378.771	378.771	∞
100	94.641	327.873	699.904	-37.203	402.636	442.548	-231.158
200	185.897	419.991	536.956	-23.393	390.090	487.446	-127.305
250	239.161	467.143	518.255	-12.778	384.125	512.475	-107.074
298.15	291.534	513.750	513.750	0.000	378.771	537.693	-94.200
300	293.529	515.560	513.756	0.541	378.573	538.678	-93.790
350	346.134	564.795	517.524	16.545	373.600	565.766	-84.434
400	395.117	614.260	526.525	35.094	369.254	593.515	-77.503
450	439.612	663.412	539.009	55.981	365.471	621.779	-72.173
500	479.464	711.833	553.878	78.977	362.179	650.455	-67.951
600	546.451	805.410	588.069	130.405	356.809	708.642	-61.691
700	599.572	893.789	625.495	187.806	352.865	767.616	-57.279
800	642.277	976.739	664.272	249.973	350.178	827.055	-54.000
900	677.143	1054.468	703.356	316.001	348.583	886.758	-51.465
1000	705.986	1127.351	742.150	385.201	347.927	946.599	-49.444
1100	730.094	1195.803	780.312	457.040	348.031	1006.475	-47.793
1200	750.413	1260.225	817.647	531.094	348.766	1066.297	-46.414
1300	767.659	1320.990	854.051	607.021	349.968	1126.048	-45.244
1400	782.386	1378.433	889.474	684.542	351.522	1185.695	-44.238
1500	795.033	1432.854	923.901	763.429	353.350	1245.224	-43.362
1600	805.953	1484.521	957.339	843.491	355.341	1304.616	-42.590
1700	815.427	1533.673	989.807	924.571	357.427	1363.860	-41.905
1800	823.688	1580.520	1021.333	1006.536	359.543	1423.035	-41.295
1900	830.924	1625.253	1051.950	1089.275	361.660	1482.047	-40.743
2000	837.289	1668.039	1081.693	1172.692	363.731	1540.971	-40.245
2100	842.913	1709.029	1110.597	1256.708	365.687	1599.781	-39.792
2200	847.902	1748.359	1138.698	1341.253	367.529	1658.504	-39.377
2300	852.344	1786.150	1166.032	1426.270	369.249	1717.145	-38.997
2400	856.313	1822.510	1192.633	1511.706	370.789	1775.673	-38.646
2500	859.873	1857.540	1218.533	1597.519	372.156	1834.238	-38.324
2600	863.076	1891.329	1243.764	1683.669	373.321	1892.652	-38.023
2700	865.967	1923.957	1268.355	1770.124	374.285	1951.086	-37.745
2800	868.584	1955.498	1292.336	1856.853	375.028	2009.509	-37.487
2900	870.961	1986.020	1315.733	1943.833	375.523	2067.862	-37.245
3000	873.124	2015.584	1338.571	2031.038	375.808	2126.225	-37.020
3100	875.098	2044.246	1360.875	2118.451	375.817	2184.518	-36.808
3200	876.905	2072.058	1382.667	2206.053	375.584	2242.877	-36.610
3300	878.561	2099.068	1403.969	2293.827	375.095	2301.279	-36.425
3400	880.084	2125.318	1424.800	2381.760	374.325	2359.628	-36.251
3500	881.487	2150.850	1445.182	2469.840	373.278	2417.988	-36.086
3600	882.781	2175.701	1465.130	2558.054	371.974	2476.455	-35.932
3700	883.978	2199.905	1484.663	2646.393	370.384	2534.978	-35.787
3800	885.088	2223.494	1503.797	2734.847	368.487	2593.495	-35.649
3900	886.117	2246.498	1522.547	2823.408	366.318	2652.023	-35.519
4000	887.075	2268.945	1540.928	2912.068	363.862	2710.728	-35.398
4100	887.966	2290.860	1558.952	3000.820	361.090	2769.435	-35.282
4200	888.798	2312.268	1576.635	3089.659	358.025	2828.205	-35.173
4300	889.574	2333.191	1593.987	3178.578	354.654	2886.976	-35.069
4400	890.301	2353.650	1611.020	3267.572	350.986	2945.907	-34.972
4500	890.982	2373.665	1627.746	3356.637	347.032	3004.974	-34.880
4600	891.620	2393.255	1644.175	3445.767	342.750	3064.136	-34.794
4700	892.220	2412.437	1660.318	3534.959	338.150	3123.299	-34.711
4800	892.784	2431.227	1676.184	3624.210	333.273	3182.653	-34.634
4900	893.315	2449.641	1691.781	3713.515	328.057	3241.996	-34.559
5000	893.815	2467.694	1707.120	3802.872	322.579	3301.610	-34.491

3.145. 4*H*-Indeno[7,1,2-*ghi*]chrysene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-62-1
Point Group: C₁

Length: 13.84 Å
Width: 10.50 Å
Breadth: 4.554 Å
L/B Ratio: 1.319

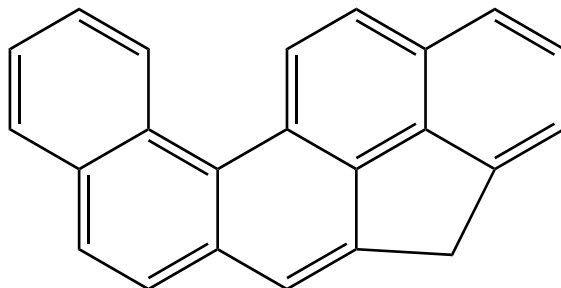
Cartesian coordinates:

C	-4.1933	1.1491	0.1504	C	-2.3116	-2.0969	0.0141	H	4.8120	2.3680	-0.3081
C	-3.4186	0.0122	0.1430	C	0.8073	2.5327	-0.2068	H	2.5529	-1.9569	0.6400
C	-2.0196	0.1925	0.0912	C	2.1634	2.5584	-0.2853	H	4.9952	-1.8163	0.6622
C	-1.3454	1.3932	0.0137	C	2.9021	1.3507	-0.1311	H	2.7043	3.4995	-0.4356
C	-2.1653	2.5423	0.0188	C	2.2305	0.1212	0.0538	H	0.2083	3.4554	-0.2623
C	-3.5415	2.4037	0.0936	C	4.3197	1.4067	-0.1207	H	-2.5239	-4.2425	-0.1625
C	0.1038	1.3027	-0.0698	C	5.0595	0.2820	0.1300	H	-0.0863	-4.5775	-0.4620
C	0.7906	0.0731	-0.0320	C	4.4011	-0.9316	0.4097	H	1.5116	-2.7424	-0.4609
C	0.0300	-1.1800	-0.0788	C	3.0326	-1.0052	0.3775	H	-1.6845	3.5289	-0.0431
C	-1.3498	-1.0600	0.0310	C	-3.6938	-1.4792	0.1353	H	-4.1630	3.3060	0.1010
C	0.4518	-2.5150	-0.2871	H	-4.1988	-1.8031	1.0630	H	-5.2853	1.1007	0.1910
C	-0.4587	-3.5590	-0.3036	H	-4.3440	-1.7680	-0.7096				
C	-1.8496	-3.3817	-0.1425	H	6.1535	0.3179	0.1335				

Table 3.145: Table of thermodynamic data as a function of temperature for 4*H*-Indeno[7,1,2-*ghi*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.908	401.917	401.917	∞
100	93.168	326.842	697.353	-37.051	425.935	465.949	-243.382
200	185.174	418.110	534.906	-23.359	413.271	511.003	-133.457
250	238.842	465.147	516.225	-12.770	407.280	536.129	-112.016
298.15	291.484	511.723	511.723	0.000	401.917	561.444	-98.361
300	293.487	513.532	511.728	0.541	401.719	562.433	-97.926
350	346.274	562.775	515.497	16.548	396.749	589.622	-87.994
400	395.370	612.266	524.500	35.106	392.413	617.471	-80.632
450	439.927	661.453	536.990	56.008	388.644	645.833	-74.965
500	479.807	709.908	551.866	79.021	385.369	674.607	-70.474
600	546.778	803.548	586.077	130.482	380.033	732.983	-63.811
700	599.839	891.973	623.526	187.913	376.119	792.141	-59.109
800	642.470	974.953	662.324	250.103	373.455	851.760	-55.613
900	677.268	1052.701	701.427	316.147	371.876	911.641	-52.909
1000	706.053	1125.595	740.237	385.357	371.229	971.657	-50.753
1100	730.116	1194.051	778.414	457.201	371.337	1031.708	-48.991
1200	750.402	1258.473	815.761	531.255	372.072	1091.706	-47.520
1300	767.623	1319.236	852.175	607.179	373.273	1151.632	-46.272
1400	782.333	1376.675	887.607	684.696	374.821	1211.455	-45.199
1500	794.969	1431.092	922.041	763.577	376.644	1271.160	-44.265
1600	805.881	1482.755	955.485	843.632	378.628	1330.728	-43.443
1700	815.351	1531.902	987.958	924.705	380.706	1390.149	-42.713
1800	823.610	1578.746	1019.489	1006.662	382.815	1449.501	-42.063
1900	830.845	1623.474	1050.109	1089.393	384.924	1508.691	-41.476
2000	837.212	1666.256	1079.855	1172.802	386.987	1567.793	-40.946
2100	842.837	1707.243	1108.762	1256.810	388.936	1626.782	-40.463
2200	847.827	1746.569	1136.865	1341.349	390.770	1685.684	-40.022
2300	852.272	1784.356	1164.201	1426.358	392.483	1744.503	-39.618
2400	856.244	1820.714	1190.803	1511.787	394.016	1803.211	-39.245
2500	859.806	1855.741	1216.704	1597.593	395.376	1861.956	-38.903
2600	863.012	1889.527	1241.936	1683.737	396.534	1920.550	-38.584
2700	865.906	1922.153	1266.529	1770.185	397.492	1979.164	-38.288
2800	868.526	1953.692	1290.510	1856.909	398.229	2037.767	-38.014
2900	870.904	1984.212	1313.907	1943.882	398.719	2096.302	-37.758
3000	873.070	2013.774	1336.746	2031.082	398.998	2154.845	-37.518
3100	875.047	2042.434	1359.050	2118.490	399.001	2213.319	-37.293
3200	876.855	2070.245	1380.843	2206.086	398.764	2271.859	-37.084
3300	878.514	2097.253	1402.145	2293.856	398.269	2330.443	-36.887
3400	880.039	2123.502	1422.977	2381.784	397.495	2388.974	-36.701
3500	881.443	2149.033	1443.359	2469.859	396.444	2447.515	-36.526
3600	882.740	2173.882	1463.307	2558.069	395.135	2506.164	-36.363
3700	883.939	2198.085	1482.840	2646.404	393.542	2564.869	-36.209
3800	885.050	2221.673	1501.974	2734.854	391.641	2623.568	-36.063
3900	886.081	2244.676	1520.724	2823.411	389.468	2682.278	-35.924
4000	887.039	2267.122	1539.105	2912.068	387.008	2741.166	-35.795
4100	887.932	2289.036	1557.130	3000.817	384.233	2800.054	-35.672
4200	888.765	2310.443	1574.812	3089.652	381.164	2859.007	-35.556
4300	889.543	2331.366	1592.164	3178.568	377.790	2917.961	-35.445
4400	890.271	2351.824	1609.197	3267.559	374.119	2977.075	-35.342
4500	890.953	2371.839	1625.923	3356.621	370.162	3036.323	-35.244
4600	891.592	2391.428	1642.352	3445.748	365.877	3095.669	-35.152
4700	892.193	2410.609	1658.495	3534.938	361.275	3155.014	-35.063
4800	892.758	2429.399	1674.360	3624.186	356.395	3214.551	-34.981
4900	893.290	2447.813	1689.958	3713.488	351.176	3274.077	-34.901
5000	893.791	2465.865	1705.296	3802.843	345.696	3333.874	-34.828

3.146. 1*H*-Dibenz[*bc,l*]aceanthrylene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-61-0
Point Group: C₁

Length: 14.61 Å
Width: 9.346 Å
Breadth: 4.563 Å
L/B Ratio: 1.563

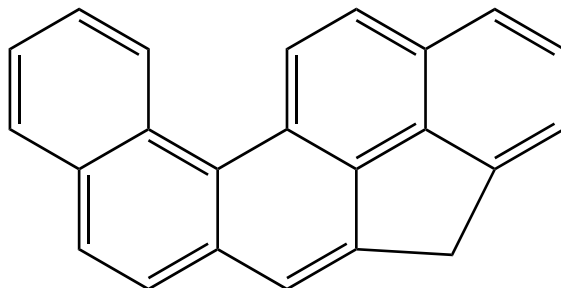
Cartesian coordinates:

C	-4.1848	-1.8619	0.1395	C	-0.3830	-1.8238	0.2538	H	5.7693	0.4806	0.3354
C	-2.8123	-1.5122	0.1269	C	-1.6506	-2.3420	0.2785	H	1.7826	-2.3268	-0.6274
C	-2.5503	-0.1603	-0.0226	C	2.2932	2.4735	0.1753	H	4.0164	-3.3283	-0.6167
C	-3.5101	0.8761	-0.1311	C	3.5017	1.8708	0.2788	H	4.4148	2.4554	0.4395
C	-4.8303	0.5063	-0.1120	C	3.6091	0.4522	0.1380	H	2.2114	3.5660	0.2267
C	-5.1414	-0.8732	0.0195	C	2.4520	-0.3313	-0.0558	H	-0.0828	3.5559	-0.0899
C	-1.2346	0.3670	-0.0469	C	4.8908	-0.1467	0.1451	H	-1.8031	-3.4158	0.4340
C	-1.3054	1.7871	-0.1370	C	5.0330	-1.4906	-0.0950	H	0.4588	-2.5095	0.4188
C	-2.7647	2.1933	-0.2263	C	3.8958	-2.2664	-0.3776	H	-5.6370	1.2408	-0.1902
C	-0.1274	2.4616	-0.0721	C	2.6440	-1.6999	-0.3639	H	-6.1999	-1.1564	0.0302
C	1.0915	1.7072	0.0259	H	-2.9805	2.7132	-1.1770	H	-4.4745	-2.9121	0.2464
C	1.1481	0.2953	0.0081	H	-3.0462	2.8790	0.5927				
C	-0.1023	-0.4219	0.0562	H	6.0220	-1.9595	-0.0862				

Table 3.146: Table of thermodynamic data as a function of temperature for 1*H*-Dibenz[*bc,l*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.689	401.453	401.453	∞
100	92.034	326.090	695.069	-36.898	425.624	465.714	-243.259
200	184.433	416.631	533.173	-23.308	412.858	510.886	-133.427
250	238.349	463.532	514.528	-12.749	406.837	536.090	-112.007
298.15	291.105	510.032	510.032	0.000	401.453	561.484	-98.368
300	293.111	511.839	510.038	0.540	401.254	562.476	-97.934
350	345.933	561.028	513.802	16.529	396.267	589.752	-88.014
400	395.030	610.474	522.796	35.071	391.914	617.689	-80.660
450	439.582	659.620	535.273	55.956	388.128	646.142	-75.001
500	479.461	708.039	550.136	78.951	384.835	675.008	-70.516
600	546.454	801.617	584.319	130.379	379.466	733.575	-63.862
700	599.557	889.995	621.739	187.779	375.521	792.929	-59.168
800	642.239	972.941	660.511	249.944	372.832	852.747	-55.677
900	677.085	1050.664	699.590	315.967	371.232	912.830	-52.978
1000	705.912	1123.541	738.380	385.161	370.569	973.051	-50.826
1100	730.009	1191.985	776.538	456.992	370.665	1033.308	-49.067
1200	750.322	1256.399	813.869	531.037	371.391	1093.513	-47.598
1300	767.564	1317.157	850.269	606.954	372.584	1153.647	-46.353
1400	782.290	1374.592	885.688	684.466	374.128	1213.678	-45.282
1500	794.939	1429.007	920.111	763.343	375.947	1273.591	-44.349
1600	805.860	1480.668	953.546	843.396	377.928	1333.368	-43.529
1700	815.338	1529.814	986.010	924.467	380.005	1392.997	-42.801
1800	823.603	1576.657	1017.533	1006.423	382.112	1452.558	-42.151
1900	830.842	1621.385	1048.146	1089.153	384.221	1511.957	-41.566
2000	837.211	1664.167	1077.886	1172.563	386.284	1571.268	-41.036
2100	842.839	1705.154	1106.786	1256.571	388.233	1630.466	-40.555
2200	847.831	1744.480	1134.885	1341.109	390.067	1689.577	-40.115
2300	852.277	1782.267	1162.216	1426.119	391.781	1748.605	-39.711
2400	856.250	1818.626	1188.813	1511.549	393.314	1807.522	-39.339
2500	859.813	1853.653	1214.711	1597.355	394.675	1866.476	-38.997
2600	863.020	1887.439	1239.939	1683.500	395.834	1925.279	-38.679
2700	865.914	1920.065	1264.528	1769.949	396.793	1984.102	-38.384
2800	868.534	1951.604	1288.507	1856.673	397.530	2042.914	-38.110
2900	870.912	1982.124	1311.901	1943.648	398.021	2101.657	-37.854
3000	873.078	2011.687	1334.737	2030.849	398.301	2160.409	-37.615
3100	875.055	2040.347	1357.039	2118.257	398.305	2219.092	-37.391
3200	876.863	2068.158	1378.829	2205.854	398.068	2277.840	-37.181
3300	878.522	2095.167	1400.129	2293.624	397.575	2336.633	-36.985
3400	880.046	2121.416	1420.959	2381.554	396.801	2395.372	-36.800
3500	881.451	2146.947	1441.338	2469.630	395.751	2454.122	-36.625
3600	882.747	2171.797	1461.285	2557.840	394.443	2512.979	-36.462
3700	883.946	2195.999	1480.817	2646.176	392.850	2571.893	-36.308
3800	885.057	2219.588	1499.949	2734.627	390.950	2630.800	-36.162
3900	886.087	2242.591	1518.697	2823.185	388.778	2689.719	-36.024
4000	887.046	2265.037	1537.077	2911.842	386.319	2748.815	-35.895
4100	887.939	2286.952	1555.100	3000.592	383.544	2807.912	-35.773
4200	888.771	2308.359	1572.781	3089.428	380.476	2867.074	-35.657
4300	889.549	2329.281	1590.131	3178.344	377.102	2926.236	-35.546
4400	890.277	2349.740	1607.164	3267.336	373.432	2985.558	-35.442
4500	890.958	2369.755	1623.889	3356.398	369.476	3045.015	-35.345
4600	891.598	2389.344	1640.317	3445.526	365.191	3104.569	-35.253
4700	892.198	2408.526	1656.458	3534.716	360.589	3164.123	-35.165
4800	892.763	2427.315	1672.323	3623.964	355.710	3223.867	-35.082
4900	893.295	2445.729	1687.919	3713.268	350.492	3283.602	-35.003
5000	893.796	2463.781	1703.257	3802.622	345.012	3343.607	-34.930

3.147. 4*H*-Benzo[*c*]cyclopenta[*mno*]chrysene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-56-3
Point Group: C₁

Length: 14.61 Å
Width: 9.349 Å
Breadth: 4.562 Å
L/B Ratio: 1.562

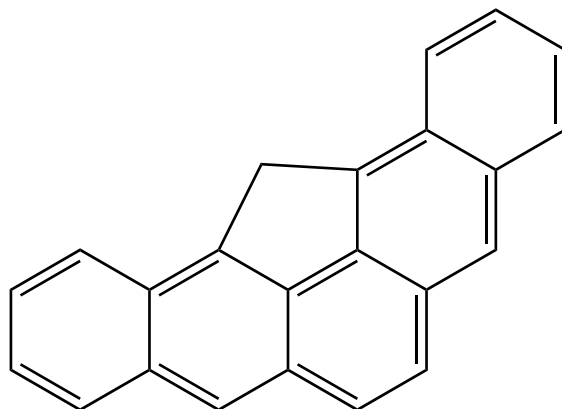
Cartesian coordinates:

C	-1.2348	-0.3679	0.0386	C	1.1480	-0.2955	-0.0087	H	5.7698	-0.4801	-0.3308
C	-1.3054	-1.7877	0.1329	C	1.0918	-1.7076	-0.0240	H	1.7817	2.3277	0.6262
C	-2.7650	-2.1939	0.2212	C	-0.1270	-2.4620	0.0744	H	4.0150	3.3293	0.6155
C	-3.5100	-0.8765	0.1276	C	-0.1024	0.4213	-0.0609	H	4.4155	-2.4553	-0.4354
C	-2.5504	0.1595	0.0148	C	-1.6505	2.3419	-0.2801	H	2.2124	-3.5664	-0.2204
C	5.0324	1.4915	0.0961	C	-0.3829	1.8235	-0.2566	H	-0.0822	-3.5562	0.0978
C	4.8907	0.1472	-0.1428	C	-2.8122	1.5120	-0.1292	H	-1.8031	3.4162	-0.4316
C	2.6431	1.7003	0.3632	C	-4.8301	-0.5056	0.1182	H	0.4587	2.5097	-0.4210
C	3.8949	2.2672	0.3773	C	-5.1411	0.8741	-0.0097	H	-5.6363	-1.2401	0.2022
C	2.4518	0.3315	0.0559	C	-4.1845	1.8624	-0.1341	H	-6.1994	1.1581	-0.0133
C	3.6093	-0.4520	-0.1362	H	-2.9808	-2.7158	1.1706	H	-4.4746	2.9129	-0.2378
C	3.5022	-1.8708	-0.2758	H	-3.0459	-2.8769	-0.6002				
C	2.2939	-2.4737	-0.1714	H	6.0215	1.9603	0.0879				

Table 3.147: Table of thermodynamic data as a function of temperature for 4*H*-Benzo[*c*]cyclopenta[*mno*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.689	401.462	401.462	∞
100	92.033	326.077	695.056	-36.898	425.633	465.724	-243.264
200	184.434	416.617	533.159	-23.308	412.866	510.897	-133.430
250	238.351	463.518	514.515	-12.749	406.846	536.102	-112.010
298.15	291.108	510.019	510.019	0.000	401.462	561.497	-98.370
300	293.114	511.826	510.025	0.540	401.263	562.489	-97.936
350	345.936	561.015	513.789	16.529	396.276	589.765	-88.016
400	395.034	610.461	522.783	35.071	391.923	617.703	-80.662
450	439.586	659.608	535.260	55.956	388.137	646.157	-75.002
500	479.465	708.027	550.123	78.952	384.845	675.024	-70.518
600	546.458	801.606	584.306	130.380	379.476	733.591	-63.863
700	599.561	889.985	621.726	187.781	375.532	792.946	-59.169
800	642.242	972.931	660.499	249.946	372.843	852.765	-55.679
900	677.087	1050.655	699.578	315.969	371.243	912.849	-52.979
1000	705.914	1123.532	738.368	385.163	370.580	973.071	-50.827
1100	730.011	1191.976	776.526	456.994	370.676	1033.329	-49.068
1200	750.323	1256.391	813.858	531.039	371.402	1093.535	-47.599
1300	767.565	1317.148	850.258	606.957	372.596	1153.670	-46.354
1400	782.291	1374.584	885.677	684.469	374.140	1213.702	-45.283
1500	794.940	1428.998	920.101	763.346	375.959	1273.615	-44.350
1600	805.861	1480.660	953.535	843.399	377.940	1333.393	-43.530
1700	815.339	1529.806	986.000	924.470	380.017	1393.024	-42.802
1800	823.603	1576.648	1017.523	1006.427	382.124	1452.585	-42.152
1900	830.842	1621.377	1048.136	1089.157	384.233	1511.985	-41.567
2000	837.212	1664.159	1077.876	1172.566	386.296	1571.297	-41.037
2100	842.840	1705.145	1106.777	1256.574	388.245	1630.495	-40.556
2200	847.832	1744.472	1134.875	1341.113	390.080	1689.607	-40.116
2300	852.277	1782.259	1162.206	1426.123	391.793	1748.636	-39.712
2400	856.250	1818.617	1188.804	1511.553	393.326	1807.554	-39.340
2500	859.814	1853.645	1214.701	1597.359	394.688	1866.508	-38.998
2600	863.020	1887.431	1239.929	1683.503	395.846	1925.312	-38.679
2700	865.914	1920.057	1264.519	1769.953	396.805	1984.136	-38.385
2800	868.534	1951.596	1288.497	1856.677	397.543	2042.949	-38.111
2900	870.913	1982.116	1311.892	1943.651	398.033	2101.693	-37.855
3000	873.078	2011.679	1334.728	2030.853	398.313	2160.446	-37.616
3100	875.055	2040.339	1357.029	2118.261	398.317	2219.129	-37.391
3200	876.863	2068.150	1378.820	2205.858	398.081	2277.879	-37.182
3300	878.522	2095.158	1400.120	2293.628	397.587	2336.672	-36.986
3400	880.047	2121.408	1420.950	2381.558	396.814	2395.412	-36.800
3500	881.451	2146.939	1441.329	2469.634	395.763	2454.163	-36.626
3600	882.747	2171.788	1461.276	2557.844	394.455	2513.021	-36.462
3700	883.946	2195.991	1480.808	2646.180	392.862	2571.935	-36.308
3800	885.057	2219.580	1499.940	2734.631	390.962	2630.844	-36.163
3900	886.088	2242.583	1518.688	2823.188	388.790	2689.763	-36.025
4000	887.046	2265.029	1537.067	2911.846	386.331	2748.860	-35.896
4100	887.939	2286.943	1555.091	3000.595	383.556	2807.958	-35.773
4200	888.771	2308.351	1572.772	3089.431	380.488	2867.120	-35.657
4300	889.549	2329.273	1590.123	3178.348	377.115	2926.283	-35.547
4400	890.277	2349.732	1607.155	3267.340	373.444	2985.606	-35.443
4500	890.959	2369.747	1623.880	3356.402	369.488	3045.064	-35.345
4600	891.598	2389.336	1640.308	3445.530	365.204	3104.618	-35.253
4700	892.199	2408.517	1656.449	3534.720	360.602	3164.173	-35.165
4800	892.763	2427.307	1672.314	3623.968	355.723	3223.919	-35.083
4900	893.295	2445.721	1687.910	3713.272	350.504	3283.655	-35.003
5000	893.796	2463.773	1703.248	3802.626	345.025	3343.660	-34.930

3.148. 1*H*-Cyclopenta[*rst*]pentaphene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-59-6
Point Group: C_{2v}

Length: 15.34 Å
Width: 9.597 Å
Breadth: 4.178 Å
L/B Ratio: 1.599

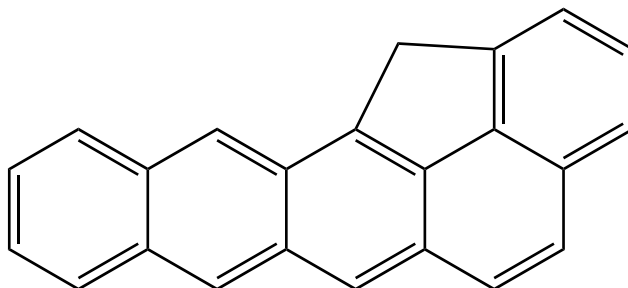
Cartesian coordinates:

C	0.0225	1.5984	-0.0027	C	0.6359	-3.0695	0.0048	H	6.4871	1.0573	-0.0058
C	1.2011	0.6383	-0.0014	C	-0.7225	-3.0503	0.0054	H	5.4224	-1.1798	-0.0030
C	0.7051	-0.6579	0.0017	C	-1.4888	-1.8133	0.0040	H	2.6175	2.9517	-0.0047
C	-0.7235	-0.6377	0.0021	C	-2.8604	-1.6282	0.0030	H	3.4693	-2.5862	0.0002
C	-1.1825	0.6719	-0.0005	C	-2.5779	0.8557	-0.0002	H	1.1767	-4.0225	0.0067
C	4.6057	2.1378	-0.0050	C	-3.3983	-0.3118	0.0016	H	-1.2899	-3.9877	0.0076
C	5.3963	0.9611	-0.0043	C	-4.8145	-0.1352	0.0015	H	-3.5410	-2.4872	0.0031
C	4.8087	-0.2714	-0.0027	C	-5.3670	1.1134	0.0006	H	-5.4537	-1.0259	0.0017
C	3.2433	2.0523	-0.0045	C	-4.5434	2.2672	-0.0008	H	-6.4545	1.2404	0.0001
C	2.6011	0.7826	-0.0026	C	-3.1839	2.1431	-0.0015	H	-5.0143	3.2556	-0.0014
C	3.3881	-0.4077	-0.0014	H	0.0315	2.2520	-0.8935	H	-2.5328	3.0244	-0.0023
C	2.8132	-1.7084	0.0008	H	0.0322	2.2552	0.8857				
C	1.4369	-1.8546	0.0029	H	5.1045	3.1124	-0.0061				

Table 3.148: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-43.133	401.121	401.121	∞
100	93.855	321.871	694.556	-37.268	424.922	465.433	-243.112
200	186.369	413.794	531.189	-23.479	412.356	510.951	-133.444
250	240.086	461.106	512.417	-12.828	406.427	536.286	-112.048
298.15	292.638	507.895	507.895	0.000	401.121	561.790	-98.421
300	294.636	509.711	507.900	0.543	400.926	562.786	-97.988
350	347.250	559.119	511.682	16.603	396.009	590.162	-88.075
400	396.158	608.728	520.713	35.206	391.717	618.191	-80.726
450	440.547	657.998	533.235	56.143	387.984	646.728	-75.069
500	480.294	706.511	548.145	79.183	384.736	675.673	-70.586
600	547.107	800.223	582.417	130.684	379.440	734.384	-63.933
700	600.112	888.694	619.916	188.145	375.555	793.873	-59.238
800	642.740	971.710	658.758	250.362	372.918	853.817	-55.747
900	677.555	1049.491	697.899	316.433	371.367	914.021	-53.047
1000	706.359	1122.416	736.743	385.673	370.749	974.357	-50.894
1100	730.437	1190.902	774.949	457.548	370.889	1034.724	-49.134
1200	750.729	1255.352	812.324	531.634	371.657	1095.035	-47.665
1300	767.951	1316.141	848.763	607.591	372.890	1155.272	-46.418
1400	782.657	1373.605	884.219	685.141	374.471	1215.404	-45.346
1500	795.285	1428.044	918.675	764.054	376.326	1275.414	-44.413
1600	806.186	1479.727	952.139	844.140	378.341	1335.286	-43.592
1700	815.644	1528.892	984.632	925.243	380.449	1395.009	-42.863
1800	823.890	1575.752	1016.180	1007.229	382.586	1454.661	-42.212
1900	831.111	1620.495	1046.818	1089.987	384.723	1514.149	-41.626
2000	837.464	1663.290	1076.579	1173.422	386.812	1573.549	-41.096
2100	843.076	1704.289	1105.501	1257.455	388.785	1632.834	-40.614
2200	848.054	1743.626	1133.619	1342.016	390.643	1692.030	-40.173
2300	852.486	1781.423	1160.968	1427.047	392.378	1751.144	-39.769
2400	856.447	1817.790	1187.583	1512.498	393.931	1810.145	-39.396
2500	859.998	1852.825	1213.496	1598.323	395.312	1869.181	-39.054
2600	863.194	1886.618	1238.739	1684.485	396.488	1928.067	-38.735
2700	866.078	1919.250	1263.342	1770.951	397.464	1986.972	-38.439
2800	868.689	1950.796	1287.334	1857.692	398.217	2045.864	-38.165
2900	871.059	1981.321	1310.741	1944.681	398.723	2104.688	-37.909
3000	873.217	2010.888	1333.589	2031.897	399.017	2163.520	-37.669
3100	875.186	2039.553	1355.902	2119.318	399.035	2222.283	-37.444
3200	876.988	2067.368	1377.703	2206.928	398.811	2281.110	-37.235
3300	878.640	2094.380	1399.013	2294.711	398.329	2339.982	-37.038
3400	880.159	2120.633	1419.853	2382.652	397.567	2398.800	-36.852
3500	881.557	2146.167	1440.242	2470.738	396.528	2457.628	-36.677
3600	882.849	2171.020	1460.198	2558.960	395.230	2516.563	-36.514
3700	884.043	2195.225	1479.738	2647.305	393.647	2575.554	-36.360
3800	885.149	2218.816	1498.878	2735.765	391.757	2634.539	-36.214
3900	886.176	2241.822	1517.634	2824.332	389.593	2693.535	-36.075
4000	887.130	2264.270	1536.021	2912.998	387.143	2752.707	-35.946
4100	888.019	2286.187	1554.051	3001.756	384.376	2811.881	-35.823
4200	888.849	2307.596	1571.739	3090.600	381.316	2871.119	-35.707
4300	889.623	2328.520	1589.096	3179.524	377.950	2930.357	-35.596
4400	890.348	2348.980	1606.134	3268.523	374.287	2989.755	-35.492
4500	891.027	2368.997	1622.865	3357.592	370.338	3049.288	-35.394
4600	891.663	2388.588	1639.299	3446.727	366.060	3108.918	-35.302
4700	892.261	2407.770	1655.446	3535.923	361.465	3168.547	-35.214
4800	892.824	2426.561	1671.316	3625.178	356.592	3228.367	-35.131
4900	893.353	2444.976	1686.918	3714.487	351.379	3288.178	-35.052
5000	893.852	2463.030	1702.260	3803.847	345.906	3348.258	-34.978

3.149. 1*H*-Indeno[2,1,7-*gra*]naphthacene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-63-2
Point Group: C_s

Length: 15.54 Å
Width: 9.274 Å
Breadth: 4.179 Å
L/B Ratio: 1.675

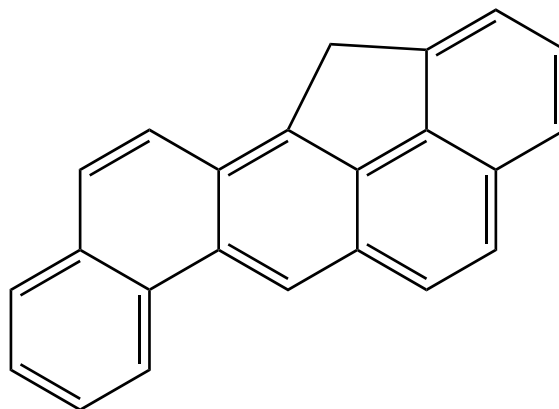
Cartesian coordinates:

C	-1.2520	1.9935	0.0026	C	0.8472	0.2803	0.0016	H	6.9402	-0.3998	-0.0029
C	-0.5179	0.6614	0.0020	C	1.1373	-1.1261	-0.0001	H	5.1131	-2.0850	-0.0042
C	-1.4512	-0.3558	0.0012	C	0.1078	-2.1228	-0.0001	H	4.0615	2.8049	0.0036
C	-2.7730	0.1817	0.0001	C	-1.2171	-1.7469	0.0006	H	2.7228	-2.6018	-0.0033
C	-2.7171	1.5891	0.0010	C	-2.4150	-2.5718	-0.0003	H	1.6524	2.2843	0.0061
C	5.5902	1.3058	0.0004	C	-3.6686	-2.0442	-0.0021	H	0.3925	-3.1810	-0.0015
C	5.8900	-0.0903	-0.0018	C	-3.9079	-0.6115	-0.0017	H	-2.2718	-3.6581	0.0012
C	4.8923	-1.0115	-0.0026	C	-5.1240	0.0960	-0.0029	H	-4.5466	-2.6996	-0.0039
C	4.3021	1.7359	0.0021	C	-5.1087	1.4862	-0.0019	H	-6.0738	-0.4483	-0.0040
C	3.2181	0.7942	0.0016	C	-3.9249	2.2546	0.0001	H	-6.0656	2.0202	-0.0024
C	3.5165	-0.5993	-0.0009	H	-0.9949	2.5973	-0.8864	H	-3.9790	3.3471	-0.0001
C	2.4837	-1.5306	-0.0016	H	-0.9973	2.5959	0.8929				
C	1.8928	1.2141	0.0032	H	6.4206	2.0193	0.0005				

Table 3.149: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[2,1,7-*qra*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.941	413.206	413.206	∞
100	92.794	327.028	698.274	-37.125	437.151	477.146	-249.230
200	185.624	418.244	535.420	-23.435	424.484	522.189	-136.379
250	239.661	465.425	516.677	-12.813	418.526	547.305	-114.351
298.15	292.435	512.159	512.159	0.000	413.206	572.603	-100.316
300	294.439	513.975	512.165	0.543	413.010	573.591	-99.869
350	347.192	563.364	515.945	16.597	408.088	600.755	-89.656
400	396.179	612.971	524.974	35.199	403.795	628.571	-82.081
450	440.612	662.245	537.494	56.138	400.063	656.896	-76.249
500	480.382	710.767	552.403	79.182	396.819	685.628	-71.626
600	547.212	804.497	586.676	130.693	391.533	743.914	-64.762
700	600.218	892.984	624.179	188.164	387.659	802.974	-59.917
800	642.842	976.014	663.025	250.392	385.033	862.488	-56.314
900	677.651	1053.807	702.170	316.473	383.491	922.261	-53.526
1000	706.450	1126.741	741.019	385.722	382.883	982.165	-51.302
1100	730.522	1195.236	779.230	457.606	383.032	1042.100	-49.484
1200	750.809	1259.694	816.610	531.701	383.808	1101.977	-47.967
1300	768.025	1320.489	853.054	607.665	385.048	1161.779	-46.680
1400	782.725	1377.958	888.513	685.222	386.637	1221.476	-45.573
1500	795.348	1432.401	922.974	764.141	388.498	1281.050	-44.609
1600	806.245	1484.088	956.442	844.234	390.519	1340.487	-43.761
1700	815.699	1533.257	988.938	925.342	392.633	1399.773	-43.009
1800	823.940	1580.120	1020.490	1007.333	394.776	1458.989	-42.338
1900	831.159	1624.865	1051.131	1090.096	396.917	1518.040	-41.733
2000	837.508	1667.663	1080.895	1173.536	399.010	1577.002	-41.186
2100	843.117	1708.664	1109.819	1257.573	400.988	1635.850	-40.689
2200	848.092	1748.003	1137.940	1342.139	402.850	1694.609	-40.234
2300	852.522	1785.801	1165.291	1427.173	404.589	1753.285	-39.818
2400	856.480	1822.170	1191.908	1512.627	406.145	1811.848	-39.433
2500	860.029	1857.206	1217.824	1598.456	407.529	1870.446	-39.080
2600	863.223	1891.000	1243.069	1684.621	408.708	1928.894	-38.751
2700	866.105	1923.634	1267.674	1771.090	409.687	1987.360	-38.447
2800	868.715	1955.180	1291.668	1857.833	410.443	2045.815	-38.164
2900	871.083	1985.706	1315.077	1944.825	410.951	2104.200	-37.900
3000	873.240	2015.274	1337.927	2032.043	411.248	2162.594	-37.653
3100	875.208	2043.940	1360.241	2119.467	411.268	2220.917	-37.421
3200	877.008	2071.756	1382.044	2207.079	411.046	2279.306	-37.205
3300	878.659	2098.768	1403.355	2294.863	410.566	2337.739	-37.003
3400	880.177	2125.022	1424.196	2382.806	409.806	2396.118	-36.811
3500	881.575	2150.556	1444.586	2470.895	408.769	2454.507	-36.631
3600	882.865	2175.409	1464.543	2559.118	407.473	2513.003	-36.462
3700	884.059	2199.615	1484.084	2647.465	405.892	2571.556	-36.303
3800	885.164	2223.207	1503.226	2735.926	404.003	2630.101	-36.153
3900	886.190	2246.213	1521.983	2824.495	401.841	2688.658	-36.010
4000	887.144	2268.661	1540.371	2913.162	399.392	2747.392	-35.877
4100	888.033	2290.578	1558.402	3001.921	396.627	2806.126	-35.750
4200	888.861	2311.988	1576.091	3090.767	393.568	2864.925	-35.630
4300	889.635	2332.912	1593.449	3179.692	390.203	2923.724	-35.515
4400	890.359	2353.373	1610.488	3268.692	386.541	2982.683	-35.408
4500	891.038	2373.389	1627.220	3357.762	382.593	3041.777	-35.307
4600	891.674	2392.980	1643.655	3446.898	378.316	3100.967	-35.212
4700	892.272	2412.163	1659.803	3536.096	373.722	3160.157	-35.120
4800	892.834	2430.955	1675.673	3625.351	368.850	3219.538	-35.035
4900	893.363	2449.370	1691.276	3714.661	363.638	3278.909	-34.953
5000	893.861	2467.423	1706.619	3804.023	358.166	3338.550	-34.877

3.150. 1*H*-Dibenz[*bc,j*]aceanthrylene



Other names: 1*H*-Acenaphtho[1,8-*ab*]phenanthrene
1',9-Methylene-1,2,5,6-dibenzanthracene

Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 201-42-3
Point Group: C_s

Length: 15.38 Å
Width: 8.968 Å
Breadth: 4.178 Å
L/B Ratio: 1.715

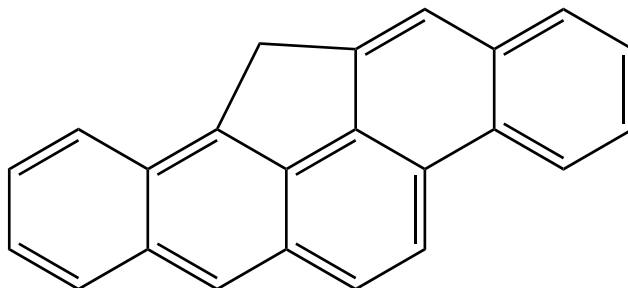
Cartesian coordinates:

C	-1.6664	2.1390	0.0074	C	0.7642	0.9781	0.0010	H	6.7486	-0.4490	0.0044
C	-0.6278	1.0273	0.0009	C	1.3937	-0.3067	-0.0018	H	5.4509	-2.5675	0.0008
C	-1.3027	-0.1985	-0.0023	C	0.6555	-1.5032	-0.0048	H	2.9661	-2.5145	-0.0029
C	-2.7081	0.0108	-0.0011	C	-0.7425	-1.4738	-0.0049	H	1.0331	3.1362	0.0046
C	-2.9916	1.3939	0.0038	C	-1.6914	-2.5671	-0.0070	H	3.5182	3.0254	0.0023
C	4.9965	0.7973	0.0030	C	-3.0406	-2.3608	-0.0066	H	1.1892	-2.4658	-0.0073
C	5.6544	-0.4137	0.0029	C	-3.6172	-1.0337	-0.0033	H	-1.2878	-3.5856	-0.0095
C	4.9218	-1.6089	0.0008	C	-4.9716	-0.6359	-0.0010	H	-3.7306	-3.2117	-0.0098
C	3.5442	-1.5778	-0.0012	C	-5.2881	0.7139	0.0025	H	-5.7621	-1.3932	-0.0026
C	3.5880	0.8438	0.0011	C	-4.3208	1.7477	0.0045	H	-6.3445	1.0053	0.0040
C	2.8478	-0.3518	-0.0010	H	-1.5644	2.7929	-0.8770	H	-4.6388	2.7943	0.0082
C	1.5607	2.1754	0.0030	H	-1.5638	2.7796	0.9015				
C	2.9096	2.1138	0.0023	H	5.5631	1.7355	0.0046				

Table 3.150: Table of thermodynamic data as a function of temperature for 1*H*-Dibenz[*bc,j*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.944	391.193	391.193	∞
100	93.125	328.092	698.786	-37.069	415.192	455.081	-237.705
200	185.280	419.306	536.227	-23.384	402.521	500.014	-130.588
250	239.123	466.388	517.526	-12.785	396.541	525.080	-109.707
298.15	291.802	513.018	513.018	0.000	391.193	550.334	-96.414
300	293.805	514.829	513.024	0.542	390.995	551.320	-95.991
350	346.537	564.118	516.796	16.563	386.040	578.443	-86.326
400	395.546	613.639	525.807	35.133	381.715	606.224	-79.163
450	440.019	662.841	538.305	56.041	377.953	634.518	-73.651
500	479.833	711.303	553.189	79.057	374.680	663.222	-69.285
600	546.739	804.940	587.412	130.517	369.343	721.458	-62.807
700	599.799	893.359	624.868	187.944	365.425	780.478	-58.239
800	642.460	976.335	663.671	250.131	362.759	839.958	-54.842
900	677.296	1054.084	702.778	316.176	361.180	899.700	-52.216
1000	706.118	1126.983	741.592	385.390	360.538	959.578	-50.122
1100	730.210	1195.446	779.772	457.242	360.654	1019.491	-48.411
1200	750.516	1259.878	817.122	531.306	361.400	1079.348	-46.982
1300	767.751	1320.650	853.540	607.243	362.613	1139.133	-45.770
1400	782.470	1378.100	888.976	684.773	364.175	1198.815	-44.727
1500	795.110	1432.526	923.414	763.668	366.011	1258.376	-43.820
1600	806.022	1484.198	956.862	843.737	368.009	1317.801	-43.021
1700	815.491	1533.354	989.340	924.824	370.102	1377.077	-42.312
1800	823.747	1580.205	1020.874	1006.795	372.224	1436.283	-41.679
1900	830.978	1624.941	1051.499	1089.539	374.347	1495.327	-41.109
2000	837.340	1667.729	1081.249	1172.962	376.423	1554.282	-40.593
2100	842.960	1708.722	1110.159	1256.983	378.384	1613.123	-40.123
2200	847.945	1748.054	1138.266	1341.533	380.230	1671.877	-39.695
2300	852.384	1785.846	1165.606	1426.553	381.955	1730.547	-39.301
2400	856.351	1822.209	1192.212	1511.994	383.498	1789.106	-38.938
2500	859.908	1857.240	1218.116	1597.810	384.870	1847.701	-38.605
2600	863.109	1891.030	1243.352	1683.964	386.037	1906.145	-38.294
2700	865.998	1923.659	1267.948	1770.421	387.005	1964.609	-38.007
2800	868.614	1955.201	1291.932	1857.154	387.751	2023.061	-37.740
2900	870.988	1985.724	1315.333	1944.136	388.249	2081.445	-37.490
3000	873.150	2015.289	1338.174	2031.345	388.536	2139.837	-37.257
3100	875.123	2043.952	1360.481	2118.760	388.547	2198.159	-37.038
3200	876.928	2071.765	1382.277	2206.364	388.317	2256.547	-36.834
3300	878.583	2098.775	1403.581	2294.140	387.830	2314.979	-36.642
3400	880.105	2125.027	1424.416	2382.076	387.062	2373.357	-36.461
3500	881.506	2150.559	1444.800	2470.157	386.018	2431.746	-36.291
3600	882.800	2175.410	1464.751	2558.373	384.715	2490.242	-36.132
3700	883.996	2199.615	1484.287	2646.714	383.128	2548.794	-35.982
3800	885.105	2223.204	1503.423	2735.170	381.232	2607.340	-35.840
3900	886.133	2246.209	1522.175	2823.732	379.065	2665.897	-35.705
4000	887.090	2268.656	1540.557	2912.394	376.610	2724.631	-35.579
4100	887.981	2290.572	1558.584	3001.148	373.840	2783.366	-35.460
4200	888.812	2311.980	1576.268	3089.988	370.776	2842.166	-35.347
4300	889.588	2332.903	1593.622	3178.908	367.406	2900.965	-35.239
4400	890.314	2353.363	1610.657	3267.904	363.740	2959.925	-35.138
4500	890.994	2373.378	1627.385	3356.970	359.787	3019.020	-35.043
4600	891.632	2392.968	1643.816	3446.101	355.506	3078.211	-34.953
4700	892.231	2412.151	1659.960	3535.295	350.907	3137.403	-34.868
4800	892.795	2430.941	1675.827	3624.546	346.032	3196.785	-34.787
4900	893.325	2449.355	1691.426	3713.853	340.816	3256.158	-34.710
5000	893.825	2467.408	1706.766	3803.210	335.340	3315.800	-34.639

3.151. 5H-Benzo[*b*]cyclopenta[*def*]chrysene



Formula: $C_{23}H_{14}$
Mass: 290.357 g/mol
CAS Number: 87308-54-1
Point Group: C_s

Length: 15.77 Å
Width: 8.983 Å
Breadth: 4.178 Å
L/B Ratio: 1.756

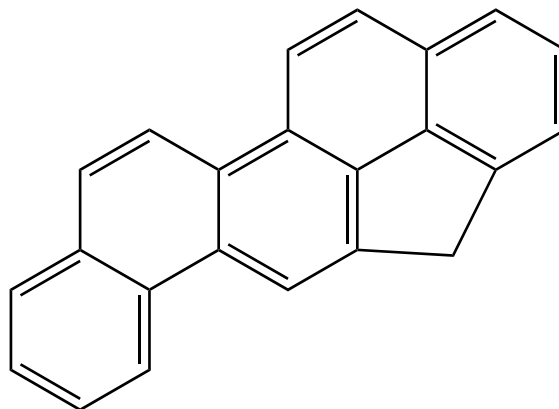
Cartesian coordinates:

C	0.6692	0.0279	0.0000	C	-0.0443	-2.6484	0.0000	H	6.5818	1.2065	-0.0000
C	0.7844	1.4521	0.0000	C	1.2713	-2.2811	0.0000	H	4.5998	2.6938	-0.0000
C	-0.6221	2.0270	0.0000	C	-1.1142	-1.6762	0.0000	H	4.0197	-2.2578	-0.0000
C	-1.5150	0.7975	0.0000	C	-2.4929	-1.8762	0.0000	H	2.2251	3.0519	0.0000
C	-0.7042	-0.3373	0.0000	C	-3.3660	-0.7663	-0.0000	H	-0.3226	-3.7080	0.0000
C	5.4143	-0.6170	-0.0000	C	-2.8981	0.5866	0.0000	H	2.0611	-3.0429	0.0000
C	5.5726	0.7816	-0.0000	C	-3.8416	1.6580	-0.0000	H	-2.9055	-2.8915	-0.0000
C	4.4733	1.6048	-0.0000	C	-5.1789	1.4017	-0.0000	H	-3.4587	2.6847	-0.0000
C	4.1568	-1.1689	-0.0000	C	-5.6537	0.0613	-0.0000	H	-5.9065	2.2198	-0.0000
C	3.0099	-0.3436	0.0000	C	-4.7814	-0.9846	-0.0000	H	-6.7346	-0.1137	-0.0000
C	3.1629	1.0673	-0.0000	H	-0.8038	2.6572	-0.8892	H	-5.1492	-2.0173	-0.0000
C	2.0393	1.9728	0.0000	H	-0.8038	2.6572	0.8892				
C	1.6832	-0.8973	0.0000	H	6.3015	-1.2584	-0.0000				

Table 3.151: Table of thermodynamic data as a function of temperature for 5*H*-Benzo[*b*]cyclopenta[*def*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-43.233	391.270	391.270	∞
100	94.398	329.481	702.420	-37.294	415.045	454.795	-237.556
200	186.429	421.598	538.994	-23.479	402.504	499.538	-130.463
250	240.079	468.914	520.223	-12.827	396.576	524.483	-109.582
298.15	292.620	515.701	515.701	0.000	391.270	549.611	-96.288
300	294.619	517.517	515.706	0.543	391.074	550.592	-95.865
350	347.247	566.923	519.488	16.602	386.157	577.578	-86.197
400	396.175	616.533	528.519	35.206	381.865	605.217	-79.032
450	440.584	665.806	541.041	56.144	378.133	633.364	-73.517
500	480.344	714.324	555.951	79.186	374.887	661.918	-69.149
600	547.168	808.047	590.225	130.693	369.597	719.848	-62.667
700	600.168	896.527	627.727	188.160	365.718	778.553	-58.095
800	642.787	979.549	666.572	250.382	363.087	837.714	-54.696
900	677.589	1057.335	705.716	316.457	361.539	897.134	-52.067
1000	706.383	1130.263	744.563	385.700	360.925	956.685	-49.971
1100	730.452	1198.750	782.772	457.577	361.067	1016.268	-48.258
1200	750.738	1263.202	820.149	531.665	361.835	1075.794	-46.827
1300	767.955	1323.992	856.590	607.622	363.069	1135.246	-45.614
1400	782.657	1381.456	892.047	685.172	364.651	1194.592	-44.570
1500	795.282	1435.895	926.505	764.084	366.505	1253.817	-43.661
1600	806.181	1487.577	959.971	844.171	368.519	1312.904	-42.861
1700	815.637	1536.742	992.464	925.273	370.627	1371.842	-42.151
1800	823.882	1583.601	1024.014	1007.258	372.764	1430.709	-41.517
1900	831.103	1628.344	1054.652	1090.015	374.900	1489.413	-40.946
2000	837.456	1671.139	1084.414	1173.450	376.987	1548.027	-40.429
2100	843.068	1712.137	1113.337	1257.481	378.960	1606.527	-39.959
2200	848.045	1751.474	1141.455	1342.042	380.817	1664.939	-39.530
2300	852.477	1789.271	1168.804	1427.072	382.551	1723.268	-39.136
2400	856.438	1825.637	1195.420	1512.522	384.103	1781.484	-38.772
2500	859.990	1860.672	1221.333	1598.346	385.483	1839.736	-38.438
2600	863.186	1894.465	1246.577	1684.508	386.659	1897.837	-38.127
2700	866.070	1927.097	1271.181	1770.973	387.634	1955.957	-37.839
2800	868.681	1958.641	1295.173	1857.713	388.386	2014.065	-37.572
2900	871.052	1989.167	1318.580	1944.701	388.891	2072.104	-37.322
3000	873.210	2018.734	1341.428	2031.916	389.185	2130.152	-37.088
3100	875.179	2047.398	1363.741	2119.337	389.202	2188.130	-36.869
3200	876.981	2075.213	1385.542	2206.946	388.977	2246.173	-36.664
3300	878.634	2102.225	1406.853	2294.728	388.495	2304.260	-36.473
3400	880.153	2128.478	1427.693	2382.669	387.732	2362.293	-36.291
3500	881.552	2154.012	1448.082	2470.755	386.692	2420.337	-36.121
3600	882.843	2178.864	1468.038	2558.975	385.394	2478.488	-35.961
3700	884.037	2203.070	1487.578	2647.320	383.811	2536.695	-35.811
3800	885.144	2226.660	1506.718	2735.780	381.920	2594.895	-35.669
3900	886.171	2249.666	1525.474	2824.346	379.756	2653.106	-35.534
4000	887.126	2272.114	1543.861	2913.012	377.305	2711.495	-35.408
4100	888.015	2294.030	1561.891	3001.769	374.538	2769.884	-35.288
4200	888.844	2315.439	1579.579	3090.613	371.477	2828.338	-35.175
4300	889.619	2336.363	1596.936	3179.536	368.111	2886.791	-35.067
4400	890.344	2356.824	1613.975	3268.535	364.447	2945.405	-34.966
4500	891.023	2376.840	1630.706	3357.603	360.498	3004.154	-34.871
4600	891.659	2396.431	1647.140	3446.738	356.219	3062.999	-34.781
4700	892.258	2415.613	1663.287	3535.934	351.624	3121.844	-34.695
4800	892.820	2434.404	1679.157	3625.188	346.751	3180.880	-34.614
4900	893.350	2452.819	1694.759	3714.497	341.538	3239.906	-34.537
5000	893.849	2470.872	1710.101	3803.857	336.064	3299.202	-34.466

3.152. 1*H*-Cyclopenta[*pqr*]picene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-60-9
Point Group: C_s

Length: 15.57 Å
Width: 8.741 Å
Breadth: 4.178 Å
L/B Ratio: 1.781

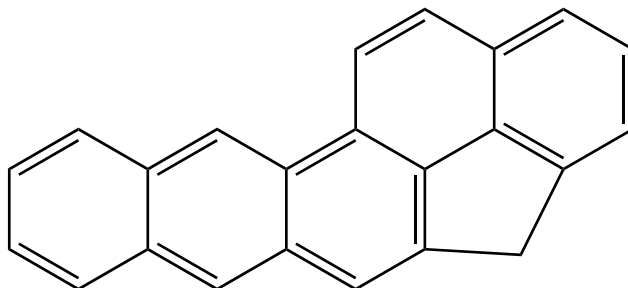
Cartesian coordinates:

C	-1.9045	2.3890	-0.0052	C	1.3926	0.2871	-0.0012	H	6.7344	0.5933	0.0083
C	-0.7513	1.3983	-0.0032	C	0.8030	-0.9928	-0.0039	H	5.6151	-1.6267	0.0035
C	-1.3055	0.0873	-0.0060	C	0.6074	1.4924	-0.0003	H	2.8948	2.5488	0.0040
C	-2.7179	0.1580	-0.0044	C	-0.6253	-1.1108	-0.0057	H	3.5986	-2.9738	-0.0018
C	-3.1437	1.5088	-0.0011	C	-1.4452	-2.2932	-0.0051	H	1.1077	-3.1392	-0.0063
C	4.8713	1.6994	0.0064	C	-2.8144	-2.2301	-0.0029	H	1.1262	2.4617	0.0027
C	5.6420	0.5218	0.0063	C	-3.5173	-0.9742	-0.0013	H	-0.9280	-3.2621	-0.0061
C	5.0234	-0.7041	0.0036	C	-4.9098	-0.7125	0.0054	H	-3.4088	-3.1502	-0.0022
C	3.5000	1.6297	0.0040	C	-5.3590	0.5941	0.0093	H	-5.6176	-1.5476	0.0076
C	2.8346	0.3798	0.0013	C	-4.4980	1.7245	0.0066	H	-6.4388	0.7809	0.0150
C	3.6112	-0.7944	0.0011	H	-1.8761	3.0380	-0.8986	H	-4.9236	2.7321	0.0110
C	2.9719	-2.0747	-0.0017	H	-1.8731	3.0478	0.8806				
C	1.6182	-2.1661	-0.0042	H	5.3754	2.6713	0.0085				

Table 3.152: Table of thermodynamic data as a function of temperature for 1*H*-Cyclopenta[*pqr*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.995	383.696	383.696	∞
100	93.565	329.453	700.165	-37.071	407.694	447.447	-233.717
200	185.237	420.817	537.653	-23.367	395.042	492.232	-128.555
250	238.937	467.873	518.967	-12.774	389.055	517.223	-108.066
298.15	291.538	514.463	514.463	0.000	383.696	542.406	-95.025
300	293.539	516.272	514.468	0.541	383.498	543.390	-94.611
350	346.232	565.517	518.237	16.548	378.529	570.442	-85.132
400	395.225	614.996	527.240	35.102	374.188	598.154	-78.109
450	439.697	664.160	539.727	55.995	370.410	626.381	-72.707
500	479.516	712.588	554.600	78.994	367.121	655.020	-68.428
600	546.440	806.169	588.797	130.423	361.753	713.131	-62.082
700	599.517	894.543	626.227	187.821	357.806	772.030	-57.608
800	642.194	977.483	665.006	249.981	355.112	831.393	-54.283
900	677.045	1055.201	704.090	316.000	353.508	891.023	-51.713
1000	705.881	1128.074	742.884	385.190	352.841	950.790	-49.663
1100	729.987	1196.516	781.044	457.019	352.935	1010.594	-47.988
1200	750.308	1260.929	818.377	531.062	353.659	1070.346	-46.590
1300	767.556	1321.685	854.779	606.978	354.851	1130.027	-45.404
1400	782.288	1379.120	890.199	684.489	356.394	1189.606	-44.384
1500	794.940	1433.535	924.624	763.366	358.213	1249.065	-43.495
1600	805.864	1485.196	958.059	843.420	360.195	1308.390	-42.714
1700	815.344	1534.342	990.524	924.491	362.272	1367.566	-42.019
1800	823.610	1581.186	1022.048	1006.448	364.380	1426.674	-41.400
1900	830.851	1625.914	1052.662	1089.179	366.490	1485.620	-40.842
2000	837.221	1668.697	1082.402	1172.589	368.553	1544.478	-40.337
2100	842.849	1709.684	1111.303	1256.599	370.503	1603.223	-39.877
2200	847.842	1749.010	1139.402	1341.138	372.339	1661.881	-39.457
2300	852.287	1786.798	1166.734	1426.149	374.054	1720.456	-39.072
2400	856.260	1823.157	1193.332	1511.580	375.588	1778.920	-38.716
2500	859.823	1858.185	1219.230	1597.387	376.950	1837.420	-38.390
2600	863.029	1891.971	1244.459	1683.532	378.109	1895.770	-38.086
2700	865.923	1924.597	1269.048	1769.982	379.069	1954.140	-37.804
2800	868.543	1956.137	1293.027	1856.708	379.808	2012.499	-37.543
2900	870.921	1986.658	1316.422	1943.683	380.299	2070.788	-37.298
3000	873.087	2016.220	1339.259	2030.885	380.580	2129.087	-37.070
3100	875.063	2044.881	1361.561	2118.294	380.585	2187.317	-36.855
3200	876.871	2072.692	1383.351	2205.892	380.349	2245.612	-36.655
3300	878.530	2099.701	1404.651	2293.663	379.856	2303.951	-36.468
3400	880.054	2125.951	1425.482	2381.593	379.083	2362.237	-36.291
3500	881.458	2151.482	1445.862	2469.670	378.034	2420.534	-36.124
3600	882.754	2176.332	1465.809	2557.881	376.726	2478.937	-35.968
3700	883.953	2200.535	1485.341	2646.218	375.134	2537.397	-35.821
3800	885.063	2224.123	1504.473	2734.669	373.235	2595.851	-35.682
3900	886.094	2247.126	1523.222	2823.227	371.063	2654.317	-35.550
4000	887.052	2269.573	1541.601	2911.885	368.605	2712.959	-35.427
4100	887.944	2291.487	1559.625	3000.636	365.831	2771.602	-35.310
4200	888.777	2312.895	1577.306	3089.472	362.763	2830.310	-35.199
4300	889.555	2333.817	1594.657	3178.389	359.390	2889.018	-35.094
4400	890.282	2354.276	1611.690	3267.381	355.720	2947.887	-34.995
4500	890.963	2374.291	1628.415	3356.444	351.765	3006.891	-34.902
4600	891.603	2393.881	1644.843	3445.573	347.481	3065.991	-34.815
4700	892.203	2413.062	1660.985	3534.763	342.879	3125.091	-34.731
4800	892.768	2431.852	1676.849	3624.012	338.001	3184.382	-34.652
4900	893.299	2450.266	1692.446	3713.316	332.783	3243.663	-34.577
5000	893.800	2468.318	1707.784	3802.671	327.304	3303.215	-34.508

3.153. 4*H*-Benzo[*b*]cyclopenta[*mno*]chrysene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 87308-55-2
Point Group: C_s

Length: 15.96 Å
Width: 8.841 Å
Breadth: 4.178 Å
L/B Ratio: 1.805

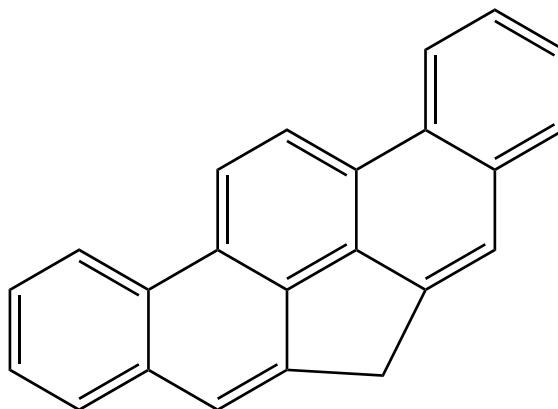
Cartesian coordinates:

C	-1.4537	0.1939	-0.0000	C	0.8809	-0.2746	0.0000	H	6.9164	0.7869	0.0000
C	-1.2824	1.6222	-0.0000	C	1.0879	1.1469	0.0000	H	4.9855	2.3532	0.0000
C	-2.6654	2.2516	-0.0000	C	-0.0169	2.0945	0.0000	H	4.2389	-2.5876	-0.0000
C	-3.6122	1.0644	-0.0000	C	-0.4799	-0.7742	-0.0000	H	2.5646	2.7199	0.0000
C	-2.8289	-0.1190	-0.0000	C	-2.2823	-2.4425	0.0000	H	1.8038	-2.2189	-0.0000
C	5.6770	-0.9966	-0.0000	C	-0.9435	-2.1297	-0.0000	H	0.2108	3.1656	0.0000
C	5.8889	0.4086	0.0000	C	-3.2931	-1.4266	0.0000	H	-2.6026	-3.4900	0.0000
C	4.8310	1.2683	0.0000	C	-4.9716	0.9034	0.0000	H	-0.1916	-2.9289	-0.0000
C	4.4123	-1.5056	-0.0000	C	-5.4941	-0.4210	0.0000	H	-5.6560	1.7565	0.0000
C	3.2823	-0.6319	-0.0000	C	-4.7076	-1.5533	0.0000	H	-6.5842	-0.5335	0.0000
C	3.4928	0.7678	0.0000	H	-2.8182	2.8891	-0.8892	H	-5.1594	-2.5504	0.0000
C	2.3882	1.6366	0.0000	H	-2.8182	2.8891	0.8892				
C	1.9696	-1.1328	-0.0000	H	6.5470	-1.6612	-0.0000				

Table 3.153: Table of thermodynamic data as a function of temperature for 4*H*-Benzo[*b*]cyclopenta[*mno*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-43.050	390.771	390.771	∞
100	93.429	329.822	701.083	-37.126	414.713	454.430	-237.365
200	185.540	421.215	538.292	-23.415	402.068	499.179	-130.370
250	239.443	468.361	519.566	-12.801	396.102	524.148	-109.512
298.15	292.169	515.052	515.052	0.000	390.771	549.305	-96.234
300	294.173	516.865	515.058	0.542	390.574	550.288	-95.812
350	346.925	566.213	518.834	16.583	385.638	577.308	-86.157
400	395.930	615.785	527.856	35.172	381.332	604.983	-79.001
450	440.387	665.032	540.367	56.099	377.589	633.168	-73.495
500	480.180	713.531	555.266	79.133	374.334	661.761	-69.132
600	547.046	807.228	589.519	130.625	369.030	719.772	-62.660
700	600.076	895.692	627.004	188.081	365.141	778.560	-58.096
800	642.717	978.704	665.835	250.295	362.501	837.805	-54.702
900	677.538	1056.482	704.966	316.365	360.947	897.309	-52.077
1000	706.346	1129.405	743.802	385.603	360.328	956.946	-49.985
1100	730.426	1197.890	782.002	457.477	360.467	1016.615	-48.274
1200	750.721	1262.340	819.372	531.562	361.234	1076.227	-46.846
1300	767.944	1323.128	855.806	607.519	362.466	1135.765	-45.635
1400	782.651	1380.591	891.258	685.067	364.047	1195.198	-44.592
1500	795.279	1435.030	925.711	763.979	365.901	1254.510	-43.685
1600	806.181	1486.713	959.172	844.066	367.915	1313.683	-42.886
1700	815.640	1535.878	991.662	925.168	370.023	1372.707	-42.177
1800	823.886	1582.737	1023.208	1007.153	372.160	1431.661	-41.545
1900	831.108	1627.480	1053.843	1089.911	374.296	1490.451	-40.975
2000	837.461	1670.275	1083.602	1173.346	376.384	1549.152	-40.459
2100	843.073	1711.274	1112.522	1257.378	378.358	1607.738	-39.989
2200	848.051	1750.611	1140.638	1341.939	380.215	1666.236	-39.561
2300	852.484	1788.408	1167.986	1426.970	381.950	1724.651	-39.167
2400	856.444	1824.774	1194.599	1512.420	383.503	1782.954	-38.804
2500	859.996	1859.809	1220.511	1598.246	384.883	1841.292	-38.471
2600	863.192	1893.602	1245.753	1684.408	386.059	1899.479	-38.160
2700	866.076	1926.235	1270.355	1770.874	387.035	1957.686	-37.873
2800	868.687	1957.780	1294.346	1857.614	387.788	2015.880	-37.606
2900	871.057	1988.305	1317.752	1944.603	388.293	2074.005	-37.356
3000	873.215	2017.872	1340.599	2031.818	388.588	2132.139	-37.123
3100	875.184	2046.537	1362.912	2119.240	388.605	2190.203	-36.904
3200	876.986	2074.352	1384.712	2206.850	388.381	2248.332	-36.700
3300	878.639	2101.364	1406.021	2294.632	387.899	2306.506	-36.508
3400	880.157	2127.617	1426.860	2382.573	387.137	2364.625	-36.327
3500	881.556	2153.151	1447.248	2470.659	386.098	2422.755	-36.157
3600	882.848	2178.004	1467.203	2558.880	384.800	2480.991	-35.998
3700	884.042	2202.209	1486.743	2647.226	383.217	2539.284	-35.848
3800	885.148	2225.800	1505.883	2735.686	381.326	2597.570	-35.705
3900	886.175	2248.806	1524.638	2824.253	379.163	2655.868	-35.571
4000	887.130	2271.254	1543.024	2912.918	376.713	2714.342	-35.445
4100	888.019	2293.170	1561.054	3001.676	373.946	2772.818	-35.325
4200	888.848	2314.579	1578.741	3090.520	370.886	2831.357	-35.212
4300	889.622	2335.504	1596.098	3179.444	367.520	2889.897	-35.105
4400	890.347	2355.964	1613.136	3268.443	363.857	2948.597	-35.004
4500	891.026	2375.980	1629.867	3357.512	359.908	3007.431	-34.909
4600	891.663	2395.571	1646.300	3446.647	355.629	3066.362	-34.819
4700	892.261	2414.754	1662.447	3535.843	351.034	3125.294	-34.733
4800	892.823	2433.545	1678.316	3625.098	346.161	3184.415	-34.653
4900	893.353	2451.960	1693.918	3714.407	340.948	3243.527	-34.576
5000	893.852	2470.013	1709.260	3803.767	335.475	3302.909	-34.505

3.154. 6*H*-Cyclopenta[*ghi*]picene



Other names: 1,2,7,8-Dibenzo-4,5-phenanthrylenemethane

Formula: C₂₃H₁₄

Mass: 290.357 g/mol

CAS Number: 195-90-4

Point Group: C_{2v}

Length: 15.85 Å

Width: 8.747 Å

Breadth: 4.178 Å

L/B Ratio: 1.812

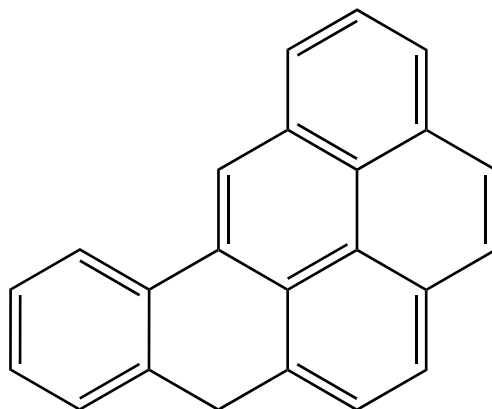
Cartesian coordinates:

C	0.6954	0.3782	-0.0000	C	-0.6444	-2.0307	0.0000	H	6.7248	0.0934	0.0000
C	1.1596	1.7348	0.0000	C	0.7336	-2.0002	0.0000	H	5.1585	2.0133	0.0000
C	-0.0585	2.6411	0.0000	C	-1.4240	-0.8346	-0.0000	H	3.4040	-2.6510	0.0000
C	-1.2352	1.6819	0.0000	C	-2.5827	1.8216	0.0000	H	2.9437	2.9349	0.0000
C	-0.7115	0.3471	-0.0000	C	-2.8590	-0.6779	0.0000	H	-1.1720	-2.9927	0.0000
C	5.1536	-1.3943	0.0000	C	-3.4057	0.6301	0.0000	H	1.3040	-2.9375	0.0000
C	5.6433	-0.0781	0.0000	C	-4.8112	0.7755	0.0000	H	-3.0702	2.8020	0.0000
C	4.7723	0.9873	0.0000	C	-5.6344	-0.3273	0.0000	H	-5.2422	1.7835	0.0000
C	3.7973	-1.6265	0.0000	C	-5.0870	-1.6205	0.0000	H	-6.7224	-0.2037	0.0000
C	2.8862	-0.5508	0.0000	C	-3.7218	-1.7927	0.0000	H	-5.7540	-2.4888	0.0000
C	3.3746	0.7801	0.0000	H	-0.0730	3.2967	-0.8892	H	-3.2844	-2.7991	0.0000
C	2.4996	1.9340	0.0000	H	-0.0730	3.2967	0.8892				
C	1.4595	-0.7708	-0.0000	H	5.8582	-2.2323	0.0000				

Table 3.154: Table of thermodynamic data as a function of temperature for 6*H*-Cyclopenta[*ghi*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-43.185	372.040	372.040	∞
100	94.431	324.245	696.461	-37.222	395.887	436.161	-227.822
200	186.010	416.231	533.373	-23.428	383.324	481.432	-125.735
250	239.548	463.440	514.642	-12.800	377.372	506.648	-105.856
298.15	292.053	510.129	510.129	0.000	372.040	532.042	-93.210
300	294.051	511.942	510.135	0.542	371.843	533.034	-92.807
350	346.689	561.261	513.910	16.573	366.898	560.301	-83.619
400	395.648	610.798	522.925	35.149	362.579	588.224	-76.813
450	440.094	660.011	535.428	56.062	358.821	616.659	-71.578
500	479.892	708.479	550.318	79.081	355.552	645.504	-67.434
600	546.781	802.126	584.549	130.546	350.219	704.023	-61.289
700	599.833	890.550	622.013	187.976	346.305	763.323	-56.959
800	642.491	973.531	660.822	250.167	343.642	823.084	-53.741
900	677.326	1051.283	699.934	316.215	342.066	883.107	-51.253
1000	706.146	1124.185	738.753	385.432	341.427	943.265	-49.270
1100	730.238	1192.651	776.936	457.287	341.546	1003.457	-47.649
1200	750.544	1257.085	814.290	531.354	342.295	1063.594	-46.296
1300	767.778	1317.860	850.711	607.293	343.510	1123.658	-45.148
1400	782.496	1375.311	886.150	684.826	345.074	1183.618	-44.160
1500	795.134	1429.740	920.591	763.723	346.914	1243.458	-43.300
1600	806.046	1481.413	954.041	843.795	348.914	1303.161	-42.543
1700	815.514	1530.570	986.521	924.884	351.009	1362.716	-41.870
1800	823.768	1577.423	1018.057	1006.858	353.133	1422.201	-41.270
1900	830.998	1622.159	1048.684	1089.604	355.258	1481.522	-40.729
2000	837.359	1664.949	1078.435	1173.028	357.336	1540.755	-40.240
2100	842.978	1705.943	1107.347	1257.051	359.299	1599.875	-39.794
2200	847.962	1745.275	1135.456	1341.603	361.147	1658.906	-39.387
2300	852.400	1783.069	1162.797	1426.625	362.874	1717.855	-39.013
2400	856.366	1819.432	1189.404	1512.067	364.418	1776.692	-38.668
2500	859.922	1854.464	1215.310	1597.884	365.791	1835.564	-38.351
2600	863.123	1888.254	1240.546	1684.039	366.960	1894.286	-38.056
2700	866.011	1920.884	1265.143	1770.499	367.929	1953.027	-37.783
2800	868.626	1952.426	1289.129	1857.233	368.676	2011.757	-37.529
2900	870.999	1982.950	1312.530	1944.216	369.175	2070.418	-37.291
3000	873.160	2012.515	1335.373	2031.425	369.464	2129.087	-37.070
3100	875.133	2041.178	1357.681	2118.841	369.476	2187.687	-36.862
3200	876.937	2068.992	1379.477	2206.446	369.247	2246.352	-36.667
3300	878.592	2096.002	1400.783	2294.224	368.761	2305.062	-36.485
3400	880.113	2122.254	1421.618	2382.160	367.994	2363.717	-36.313
3500	881.515	2147.786	1442.003	2470.243	366.950	2422.383	-36.151
3600	882.808	2172.638	1461.955	2558.460	365.648	2481.157	-36.000
3700	884.004	2196.842	1481.491	2646.801	364.062	2539.986	-35.857
3800	885.112	2220.432	1500.627	2735.257	362.167	2598.809	-35.722
3900	886.140	2243.437	1519.380	2823.821	360.000	2657.643	-35.594
4000	887.097	2265.884	1537.763	2912.483	357.547	2716.655	-35.475
4100	887.987	2287.800	1555.791	3001.238	354.776	2775.667	-35.362
4200	888.818	2309.208	1573.475	3090.078	351.713	2834.744	-35.254
4300	889.594	2330.132	1590.830	3178.999	348.344	2893.820	-35.152
4400	890.319	2350.591	1607.865	3267.996	344.678	2953.058	-35.057
4500	890.999	2370.607	1624.593	3357.062	340.726	3012.430	-34.967
4600	891.637	2390.197	1641.025	3446.194	336.446	3071.898	-34.882
4700	892.236	2409.380	1657.169	3535.388	331.848	3131.367	-34.801
4800	892.800	2428.170	1673.037	3624.640	326.973	3191.026	-34.725
4900	893.330	2446.585	1688.636	3713.947	321.757	3250.675	-34.652
5000	893.830	2464.637	1703.976	3803.305	316.282	3310.595	-34.585

3.155. 8*H*-Dibenzo[*b,fg*]pyrene



Formula: C₂₃H₁₄
Mass: 290.357 g/mol
CAS Number: 189-71-9
Point Group: C_s

Length: 13.82 Å
Width: 10.32 Å
Breadth: 4.171 Å
L/B Ratio: 1.339

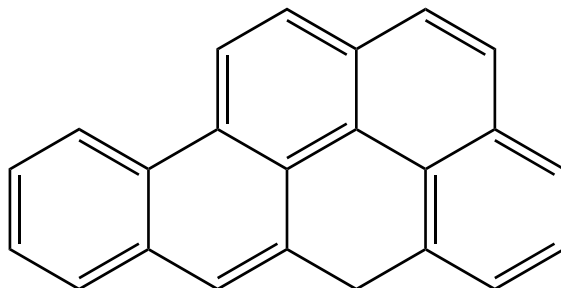
Cartesian coordinates:

C	4.3947	-1.9310	0.0000	C	-3.3740	-0.3995	0.0000	H	2.4181	-2.8065	0.0000
C	5.1344	-0.7513	0.0000	C	-4.1101	-1.5883	0.0000	H	2.8032	2.4483	0.8860
C	4.4817	0.4728	0.0000	C	-3.4577	-2.8153	-0.0000	H	2.8032	2.4483	-0.8860
C	3.0096	-1.8779	0.0000	C	-2.0696	-2.8833	0.0000	H	0.8759	4.0370	-0.0000
C	2.3370	-0.6483	0.0000	C	-1.9622	-0.4586	0.0000	H	-1.6001	4.1449	0.0000
C	3.0848	0.5357	0.0000	C	-1.3078	-1.7105	0.0000	H	-3.7819	3.0108	0.0000
C	2.4456	1.8822	-0.0000	C	0.1282	-1.7448	0.0000	H	-5.1138	0.9161	0.0000
C	0.9563	1.8811	0.0000	C	0.8730	-0.6041	0.0000	H	-5.2052	-1.5482	-0.0000
C	0.2901	3.1105	0.0000	C	0.2229	0.6896	0.0000	H	-4.0445	-3.7400	-0.0000
C	-1.0940	3.1729	0.0000	C	-1.1913	0.7487	0.0000	H	-1.5669	-3.8570	-0.0000
C	-1.8518	1.9967	0.0000	H	4.9058	-2.8990	0.0000	H	0.6271	-2.7276	0.0000
C	-3.2920	2.0303	0.0000	H	6.2285	-0.7897	0.0000				
C	-4.0181	0.8891	0.0000	H	5.0623	1.4024	-0.0000				

Table 3.155: Table of thermodynamic data as a function of temperature for 8*H*-Dibenzo[*b*,*f*g]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-42.743	337.924	337.924	∞
100	92.384	333.619	701.499	-36.788	362.205	401.542	-209.739
200	183.929	424.187	540.183	-23.199	349.438	445.954	-116.469
250	237.207	470.906	521.631	-12.681	343.376	470.785	-98.363
298.15	289.454	517.160	517.160	0.000	337.924	495.830	-86.866
300	291.443	518.957	517.165	0.537	337.722	496.809	-86.500
350	343.927	567.860	520.908	16.433	332.642	523.736	-78.162
400	392.864	617.026	529.850	34.870	328.184	551.338	-71.996
450	437.391	665.915	542.257	55.646	324.289	579.471	-67.262
500	477.335	714.105	557.039	78.533	320.888	608.028	-63.519
600	544.598	807.318	591.050	129.760	315.318	666.007	-57.980
700	598.027	895.434	628.303	186.992	311.205	724.804	-54.084
800	641.013	978.196	666.923	249.019	308.378	784.088	-51.195
900	676.117	1055.791	705.866	314.932	306.668	843.653	-48.963
1000	705.152	1128.576	744.536	384.040	305.919	903.366	-47.186
1100	729.414	1196.956	782.589	455.804	305.948	963.123	-45.734
1200	749.855	1261.325	819.828	529.796	306.621	1022.833	-44.522
1300	767.196	1322.048	856.147	605.672	307.773	1082.476	-43.494
1400	782.000	1379.460	891.495	683.151	309.284	1142.020	-42.608
1500	794.708	1433.856	925.855	762.002	311.077	1201.446	-41.837
1600	805.676	1485.504	959.233	842.034	313.037	1260.739	-41.158
1700	815.190	1534.640	991.647	923.089	315.098	1319.886	-40.554
1800	823.484	1581.475	1023.124	1005.032	317.192	1378.964	-40.016
1900	830.746	1626.198	1053.697	1087.751	319.290	1437.882	-39.529
2000	837.133	1668.975	1083.399	1171.152	321.344	1496.711	-39.089
2100	842.776	1709.958	1112.266	1255.153	323.286	1555.429	-38.688
2200	847.780	1749.282	1140.334	1339.686	325.115	1614.059	-38.322
2300	852.235	1787.068	1167.637	1424.691	326.824	1672.607	-37.985
2400	856.216	1823.424	1194.209	1510.117	328.353	1731.045	-37.674
2500	859.785	1858.450	1220.082	1595.920	329.711	1789.518	-37.389
2600	862.996	1892.235	1245.288	1682.062	330.867	1847.842	-37.123
2700	865.895	1924.860	1269.857	1768.509	331.824	1906.185	-36.877
2800	868.518	1956.399	1293.816	1855.232	332.560	1964.517	-36.648
2900	870.900	1986.919	1317.193	1942.205	333.049	2022.781	-36.433
3000	873.068	2016.481	1340.012	2029.405	333.328	2081.054	-36.234
3100	875.047	2045.141	1362.299	2116.812	333.331	2139.257	-36.045
3200	876.857	2072.952	1384.074	2204.408	333.093	2197.526	-35.870
3300	878.517	2099.960	1405.360	2292.178	332.599	2255.840	-35.706
3400	880.043	2126.209	1426.178	2380.107	331.825	2314.100	-35.551
3500	881.448	2151.740	1446.545	2468.183	330.775	2372.370	-35.405
3600	882.745	2176.590	1466.480	2556.393	329.466	2430.748	-35.269
3700	883.945	2200.792	1486.001	2644.729	327.874	2489.183	-35.140
3800	885.056	2224.381	1505.123	2733.179	325.973	2547.610	-35.019
3900	886.088	2247.384	1523.862	2821.737	323.801	2606.050	-34.903
4000	887.047	2269.830	1542.231	2910.395	321.343	2664.667	-34.796
4100	887.940	2291.745	1560.246	2999.144	318.567	2723.285	-34.694
4200	888.773	2313.152	1577.918	3087.981	315.499	2781.967	-34.598
4300	889.551	2334.074	1595.261	3176.897	312.126	2840.649	-34.506
4400	890.278	2354.533	1612.286	3265.889	308.456	2899.492	-34.421
4500	890.960	2374.548	1629.003	3354.951	304.500	2958.470	-34.340
4600	891.600	2394.137	1645.424	3444.080	300.216	3017.544	-34.265
4700	892.201	2413.319	1661.559	3533.270	295.614	3076.619	-34.192
4800	892.765	2432.109	1677.417	3622.519	290.736	3135.885	-34.125
4900	893.297	2450.522	1693.008	3711.822	285.517	3195.140	-34.060
5000	893.799	2468.574	1708.339	3801.177	280.038	3254.666	-34.001

3.156. 6*H*-Naphtho[1,2,3-*cd*]pyrene



Other names: 1',3'-Naphtha-3,4-pyrene

Formula: C₂₃H₁₄

Mass: 290.357 g/mol

CAS Number: 189-73-1

Point Group: C_s

Length: 14.12 Å

Width: 9.508 Å

Breadth: 4.171 Å

L/B Ratio: 1.485

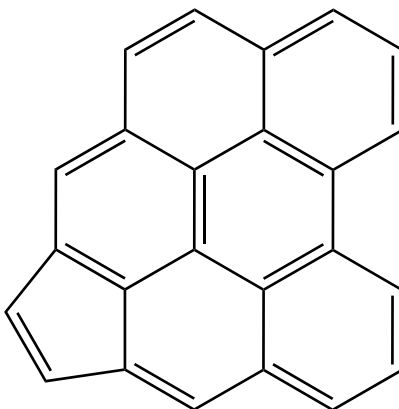
Cartesian coordinates:

C	5.1306	-0.5608	-0.0000	C	-3.4757	-0.3926	-0.0000	H	3.7616	-2.2291	0.0000
C	5.2662	0.8402	-0.0000	C	-3.2151	2.3886	0.0000	H	1.8288	2.9858	0.0000
C	4.1512	1.6427	-0.0000	C	-4.4892	1.7994	-0.0000	H	-0.1624	-3.9561	0.0000
C	3.8828	-1.1351	0.0000	C	-4.6227	0.4304	-0.0000	H	2.1181	-2.9520	0.0000
C	2.7194	-0.3308	0.0000	C	0.2746	-0.0701	0.0000	H	-4.6036	-2.2565	-0.0000
C	2.8580	1.0685	0.0000	C	0.4410	1.3551	0.0000	H	-2.5841	-3.7034	0.0000
C	1.6934	1.8970	0.0000	C	-0.7409	2.2668	0.0000	H	-3.1275	3.4809	0.0000
C	1.3980	-0.9065	0.0000	C	-2.0763	1.6044	0.0000	H	-5.3761	2.4416	-0.0000
C	-0.0304	-2.8682	0.0000	C	-2.1968	0.1952	0.0000	H	-5.6153	-0.0339	-0.0000
C	1.2182	-2.3177	0.0000	C	-1.0315	-0.6462	0.0000	H	-0.6763	2.9335	0.8857
C	-1.1826	-2.0362	0.0000	H	6.0282	-1.1877	-0.0000	H	-0.6763	2.9335	-0.8857
C	-3.5979	-1.8208	-0.0000	H	6.2677	1.2826	-0.0000				
C	-2.4948	-2.6110	0.0000	H	4.2495	2.7341	-0.0000				

Table 3.156: Table of thermodynamic data as a function of temperature for 6*H*-Naphtho[1,2,3-*cd*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-42.914	338.124	338.124	∞
100	92.981	331.882	701.282	-36.940	362.253	401.763	-209.855
200	184.706	422.892	539.323	-23.286	349.551	446.326	-116.566
250	238.107	469.799	520.704	-12.726	343.531	471.216	-98.453
298.15	290.412	516.217	516.217	0.000	338.124	496.311	-86.950
300	292.403	518.019	516.222	0.539	337.924	497.292	-86.584
350	344.892	567.072	519.976	16.483	332.892	524.261	-78.240
400	393.796	616.365	528.945	34.968	328.482	551.900	-72.069
450	438.268	665.360	541.385	55.789	324.632	580.063	-67.331
500	478.147	713.640	556.204	78.718	321.273	608.645	-63.583
600	545.275	806.988	590.288	130.020	315.778	666.664	-58.037
700	598.580	895.200	627.610	187.313	311.725	725.489	-54.136
800	641.463	978.028	666.291	249.390	308.948	784.793	-51.241
900	676.483	1055.671	705.289	315.344	307.280	844.372	-49.005
1000	705.453	1128.492	744.006	384.485	306.564	904.095	-47.224
1100	729.662	1196.897	782.101	456.276	306.620	963.860	-45.769
1200	750.062	1261.286	819.377	530.291	307.316	1023.574	-44.554
1300	767.371	1322.025	855.728	606.186	308.486	1083.220	-43.523
1400	782.148	1379.448	891.105	683.681	310.013	1142.766	-42.636
1500	794.835	1433.854	925.490	762.546	311.820	1202.193	-41.863
1600	805.786	1485.510	958.891	842.590	313.793	1261.486	-41.182
1700	815.287	1534.652	991.326	923.655	315.863	1320.631	-40.577
1800	823.568	1581.492	1022.822	1005.607	317.966	1379.708	-40.037
1900	830.820	1626.219	1053.412	1088.334	320.073	1438.624	-39.550
2000	837.200	1669.000	1083.129	1171.742	322.134	1497.451	-39.109
2100	842.835	1709.986	1112.011	1255.749	324.082	1556.166	-38.707
2200	847.833	1749.313	1140.091	1340.288	325.916	1614.794	-38.339
2300	852.283	1787.100	1167.406	1425.298	327.630	1673.339	-38.002
2400	856.260	1823.459	1193.989	1510.728	329.164	1731.773	-37.690
2500	859.825	1858.487	1219.872	1596.536	330.527	1790.242	-37.404
2600	863.033	1892.273	1245.088	1682.682	331.686	1848.562	-37.137
2700	865.929	1924.900	1269.665	1769.132	332.647	1906.902	-36.890
2800	868.550	1956.440	1293.633	1855.858	333.386	1965.230	-36.661
2900	870.929	1986.960	1317.017	1942.834	333.878	2023.490	-36.446
3000	873.095	2016.523	1339.844	2030.037	334.160	2081.758	-36.246
3100	875.072	2045.185	1362.137	2117.447	334.165	2139.957	-36.057
3200	876.880	2072.996	1383.919	2205.046	333.930	2198.222	-35.882
3300	878.539	2100.005	1405.211	2292.818	333.439	2256.531	-35.717
3400	880.063	2126.255	1426.034	2380.749	332.667	2314.786	-35.562
3500	881.467	2151.786	1446.407	2468.826	331.618	2373.053	-35.415
3600	882.763	2176.636	1466.348	2557.039	330.312	2431.426	-35.278
3700	883.962	2200.840	1485.873	2645.376	328.721	2489.855	-35.150
3800	885.072	2224.428	1505.000	2733.828	326.822	2548.279	-35.028
3900	886.103	2247.432	1523.743	2822.388	324.651	2606.714	-34.912
4000	887.061	2269.878	1542.117	2911.046	322.194	2665.325	-34.805
4100	887.953	2291.793	1560.135	2999.798	319.420	2723.938	-34.703
4200	888.786	2313.201	1577.812	3088.635	316.354	2782.616	-34.606
4300	889.563	2334.124	1595.158	3177.553	312.982	2841.293	-34.514
4400	890.290	2354.583	1612.186	3266.546	309.313	2900.131	-34.428
4500	890.972	2374.598	1628.907	3355.609	305.358	2959.104	-34.348
4600	891.611	2394.187	1645.331	3444.739	301.075	3018.173	-34.272
4700	892.211	2413.369	1661.469	3533.930	296.474	3077.243	-34.199
4800	892.775	2432.159	1677.330	3623.180	291.597	3136.503	-34.131
4900	893.307	2450.573	1692.923	3712.484	286.379	3195.754	-34.066
5000	893.808	2468.625	1708.257	3801.840	280.901	3255.274	-34.007

3.157. Indeno[5,6,7,1-*pqra*]perylene



Formula: C₂₄H₁₂
Mass: 300.352 g/mol
CAS Number: 96915-18-3
Point Group: C_s

Length: 12.83 Å
Width: 11.68 Å
Breadth: 3.890 Å
L/B Ratio: 1.098

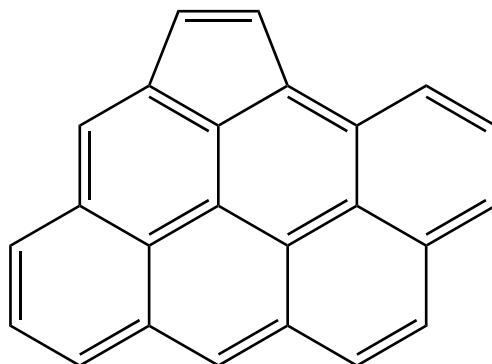
Cartesian coordinates:

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C	-3.1453	-1.5565	0.0000	C	1.0719	2.9622	0.0000	H	4.1419	3.2135	0.0000
C	-1.8664	-1.0193	0.0000	C	0.6015	-1.2789	0.0000	H	-3.2596	-2.6515	0.0000
C	-1.7300	0.3986	0.0000	C	1.7977	-2.0336	0.0000	H	-5.0274	1.2949	0.0000
C	-2.8596	1.2367	0.0000	C	3.0946	-1.3832	0.0000	H	-3.5576	3.2965	0.0000
C	-4.1410	0.6508	0.0000	C	3.1593	-0.0241	0.0000	H	-1.2979	4.3041	0.0000
C	-0.4365	1.0051	0.0000	C	-0.6797	-1.8791	0.0000	H	1.1863	4.0513	0.0000
C	-0.2445	2.3969	0.0000	C	1.6746	-3.4366	0.0000	H	2.5787	-4.0559	0.0000
C	-1.4228	3.2152	0.0000	C	0.4252	-4.0300	0.0000	H	0.3453	-5.1225	0.0000
C	-2.6650	2.6601	0.0000	C	-0.7486	-3.2660	0.0000	H	-1.7375	-3.7492	0.0000
C	0.6864	0.1438	0.0000	C	4.2053	1.0174	0.0000	H	3.9938	-2.0083	0.0000
C	1.9288	0.7184	0.0000	C	3.6288	2.2538	0.0000	H	-5.2688	-1.1768	0.0000

Table 3.157: Table of thermodynamic data as a function of temperature for Indeno[5,6,7,1-*pqra*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.345	430.062	430.062	∞
100	85.477	318.195	678.014	-35.982	450.672	481.573	-251.543
200	180.141	404.905	519.561	-22.931	439.735	516.842	-134.982
250	234.588	450.915	501.199	-12.571	434.615	536.710	-112.137
298.15	287.407	496.764	496.764	0.000	430.062	556.798	-97.547
300	289.408	498.548	496.770	0.534	429.893	557.583	-97.082
350	341.973	547.150	500.488	16.332	425.694	579.206	-86.440
400	390.643	596.040	509.377	34.665	422.037	601.384	-78.531
450	434.689	644.641	521.711	55.319	418.852	623.998	-72.430
500	474.020	692.516	536.405	78.056	416.065	646.962	-67.586
600	539.845	785.000	570.198	128.881	411.445	693.597	-60.382
700	591.698	872.267	607.182	185.559	407.943	740.920	-55.287
800	633.078	954.079	645.487	246.873	405.435	788.661	-51.493
900	666.619	1030.648	684.076	311.914	403.792	836.658	-48.557
1000	694.183	1102.355	722.357	379.998	402.900	884.808	-46.217
1100	717.092	1169.625	759.992	450.596	402.608	933.027	-44.305
1200	736.309	1232.868	796.790	523.294	402.813	981.232	-42.711
1300	752.554	1292.464	832.649	597.759	403.377	1029.416	-41.362
1400	766.382	1348.753	867.522	673.724	404.198	1077.548	-40.203
1500	778.226	1402.043	901.396	750.969	405.219	1125.617	-39.197
1600	788.428	1452.602	934.280	829.314	406.338	1173.606	-38.314
1700	797.265	1500.671	966.195	908.609	407.501	1221.503	-37.531
1800	804.957	1546.465	997.170	988.729	408.649	1269.387	-36.836
1900	811.686	1590.171	1027.240	1069.569	409.761	1317.162	-36.211
2000	817.599	1631.958	1056.439	1151.039	410.795	1364.903	-35.647
2100	822.818	1671.978	1084.804	1233.066	411.689	1412.583	-35.135
2200	827.444	1710.364	1112.372	1315.583	412.445	1460.225	-34.669
2300	831.560	1747.238	1139.178	1398.537	413.061	1507.838	-34.243
2400	835.236	1782.708	1165.258	1481.881	413.478	1555.384	-33.851
2500	838.530	1816.872	1190.643	1565.572	413.710	1603.014	-33.492
2600	841.493	1849.819	1215.366	1649.576	413.725	1650.539	-33.159
2700	844.166	1881.628	1239.457	1733.861	413.531	1698.132	-32.852
2800	846.586	1912.373	1262.944	1818.400	413.104	1745.751	-32.567
2900	848.781	1942.119	1285.854	1903.170	412.422	1793.346	-32.301
3000	850.779	1970.929	1308.212	1988.150	411.524	1840.992	-32.054
3100	852.602	1998.856	1330.043	2073.320	410.342	1888.603	-31.822
3200	854.270	2025.951	1351.368	2158.665	408.915	1936.322	-31.607
3300	855.799	2052.262	1372.211	2244.170	407.228	1984.125	-31.405
3400	857.204	2077.832	1392.590	2329.821	405.255	2031.904	-31.216
3500	858.498	2102.699	1412.525	2415.607	403.003	2079.731	-31.038
3600	859.693	2126.900	1432.035	2501.517	400.491	2127.705	-30.872
3700	860.797	2150.470	1451.135	2587.543	397.692	2175.763	-30.716
3800	861.820	2173.440	1469.842	2673.674	394.586	2223.852	-30.568
3900	862.769	2195.839	1488.171	2759.904	391.206	2271.978	-30.429
4000	863.652	2217.693	1506.137	2846.226	387.540	2320.318	-30.300
4100	864.473	2239.029	1523.753	2932.632	383.556	2368.688	-30.177
4200	865.240	2259.870	1541.033	3019.119	379.280	2417.152	-30.061
4300	865.956	2280.238	1557.988	3105.679	374.701	2465.642	-29.951
4400	866.625	2300.154	1574.630	3192.308	369.824	2514.322	-29.848
4500	867.253	2319.637	1590.970	3279.002	364.664	2563.163	-29.752
4600	867.841	2338.705	1607.018	3365.757	359.175	2612.133	-29.661
4700	868.394	2357.375	1622.785	3452.569	353.371	2661.125	-29.574
4800	868.913	2375.663	1638.280	3539.435	347.291	2710.337	-29.494
4900	869.402	2393.584	1653.512	3626.351	340.871	2759.559	-29.417
5000	869.863	2411.153	1668.490	3713.315	334.192	2809.077	-29.346

3.158. Benz[*mno*]indeno[5,6,7,1-*defg*]chrysene



Formula: C₂₄H₁₂
Mass: 300.352 g/mol
CAS Number: 96915-20-7
Point Group: C_s

Length: 12.85 Å
Width: 10.73 Å
Breadth: 3.887 Å
L/B Ratio: 1.198

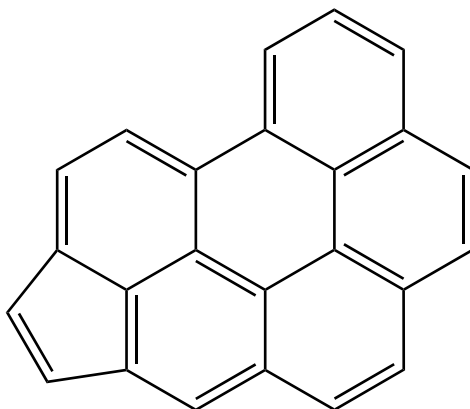
Cartesian coordinates:

C	1.9142	-0.2800	0.0000	C	-2.5433	-2.7366	0.0000	H	0.8560	4.7301	0.0000
C	2.2288	-1.6545	0.0000	C	-1.2636	-3.1681	0.0000	H	-1.7487	4.1070	0.0000
C	3.5957	-2.0104	0.0000	C	-2.1503	1.0269	0.0000	H	5.0407	1.0831	0.0000
C	4.5655	-1.0294	0.0000	C	-3.5031	1.4198	0.0000	H	5.6232	-1.3152	0.0000
C	4.2376	0.3373	0.0000	C	-4.5052	0.4722	0.0000	H	3.8754	-3.0699	0.0000
C	2.9109	0.7413	0.0000	C	-4.2080	-0.8978	0.0000	H	1.4317	-3.6785	0.0000
C	0.5463	0.0820	0.0000	C	0.2222	1.4419	0.0000	H	-1.0276	-4.2382	0.0000
C	-0.4962	-0.8419	0.0000	C	-1.0652	1.9510	0.0000	H	-3.3725	-3.4542	0.0000
C	-0.1579	-2.2330	0.0000	C	2.5303	2.1534	0.0000	H	-5.0241	-1.6289	0.0000
C	1.1677	-2.6139	0.0000	C	1.2208	2.4946	0.0000	H	-5.5538	0.7888	0.0000
C	-1.8430	-0.3668	0.0000	C	0.4205	3.7334	0.0000	H	-3.7445	2.4888	0.0000
C	-2.8894	-1.3280	0.0000	C	-0.9089	3.4145	0.0000	H	3.3291	2.9030	0.0000

Table 3.158: Table of thermodynamic data as a function of temperature for Benz[*mno*]indeno[5,6,7,1-*defg*]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-41.260	454.831	454.831	∞
100	84.819	316.308	676.128	-35.982	475.441	506.531	-264.579
200	180.242	402.827	517.599	-22.954	464.481	542.003	-141.554
250	234.846	448.879	499.218	-12.585	459.370	561.974	-117.416
298.15	287.703	494.778	494.778	0.000	454.831	582.159	-101.990
300	289.705	496.564	494.783	0.534	454.663	582.948	-101.498
350	342.245	545.210	498.505	16.347	450.477	604.669	-90.240
400	390.871	594.134	507.401	34.693	446.834	626.944	-81.869
450	434.870	642.758	519.745	55.356	443.659	649.652	-75.408
500	474.163	690.651	534.448	78.101	440.880	672.710	-70.276
600	539.938	783.156	568.258	128.939	436.271	719.530	-62.639
700	591.769	870.435	605.257	185.624	432.777	767.036	-57.236
800	633.141	952.255	643.574	246.945	430.276	814.961	-53.210
900	666.680	1028.832	682.173	311.992	428.639	863.140	-50.094
1000	694.244	1100.546	720.464	380.082	427.753	911.471	-47.609
1100	717.154	1167.822	758.107	450.686	427.467	959.870	-45.579
1200	736.370	1231.070	794.912	523.390	427.679	1008.256	-43.887
1300	752.615	1290.670	830.777	597.862	428.248	1056.619	-42.455
1400	766.442	1346.964	865.656	673.833	429.075	1104.930	-41.225
1500	778.283	1400.258	899.535	751.084	430.103	1153.178	-40.156
1600	788.483	1450.821	932.424	829.435	431.227	1201.345	-39.219
1700	797.317	1498.893	964.343	908.735	432.396	1249.420	-38.389
1800	805.007	1544.689	995.323	988.860	433.549	1297.481	-37.651
1900	811.733	1588.398	1025.396	1069.704	434.665	1345.434	-36.988
2000	817.644	1630.188	1054.598	1151.180	435.704	1393.352	-36.390
2100	822.861	1670.210	1082.967	1233.210	436.603	1441.209	-35.847
2200	827.484	1708.598	1110.538	1315.732	437.363	1489.028	-35.353
2300	831.598	1745.474	1137.348	1398.690	437.983	1536.817	-34.901
2400	835.271	1780.945	1163.430	1482.037	438.404	1584.539	-34.486
2500	838.564	1815.111	1188.818	1565.732	438.638	1632.346	-34.105
2600	841.525	1848.059	1213.544	1649.739	438.657	1680.047	-33.752
2700	844.197	1879.869	1237.637	1734.027	438.466	1727.816	-33.426
2800	846.614	1910.615	1261.126	1818.569	438.042	1775.611	-33.124
2900	848.808	1940.363	1284.038	1903.342	437.363	1823.382	-32.842
3000	850.805	1969.173	1306.398	1988.325	436.467	1871.203	-32.580
3100	852.627	1997.101	1328.230	2073.498	435.288	1918.990	-32.334
3200	854.293	2024.197	1349.558	2158.845	433.864	1966.884	-32.105
3300	855.821	2050.509	1370.402	2244.352	432.178	2014.862	-31.892
3400	857.225	2076.079	1390.783	2330.005	430.208	2062.817	-31.691
3500	858.518	2100.947	1410.720	2415.793	427.958	2110.819	-31.502
3600	859.712	2125.149	1430.231	2501.705	425.448	2158.968	-31.325
3700	860.815	2148.719	1449.332	2587.732	422.651	2207.201	-31.159
3800	861.837	2171.689	1468.041	2673.866	419.546	2255.466	-31.003
3900	862.786	2194.088	1486.371	2760.097	416.168	2303.767	-30.855
4000	863.668	2215.943	1504.338	2846.420	412.503	2352.281	-30.717
4100	864.489	2237.280	1521.956	2932.829	408.522	2400.827	-30.586
4200	865.255	2258.121	1539.236	3019.316	404.247	2449.466	-30.463
4300	865.970	2278.490	1556.192	3105.878	399.669	2498.131	-30.346
4400	866.639	2298.406	1572.835	3192.509	394.794	2546.985	-30.236
4500	867.266	2317.889	1589.176	3279.204	389.635	2596.001	-30.133
4600	867.853	2336.957	1605.226	3365.961	384.147	2645.146	-30.036
4700	868.405	2355.627	1620.994	3452.774	378.345	2694.313	-29.943
4800	868.925	2373.915	1636.490	3539.641	372.265	2743.700	-29.857
4900	869.413	2391.837	1651.723	3626.558	365.847	2793.097	-29.774
5000	869.874	2409.406	1666.702	3713.522	359.169	2842.789	-29.698

3.159. Benzo[ghi]cyclopenta[cd]perylene



Formula: C₂₄H₁₂
Mass: 300.352 g/mol
CAS Number: 190-88-5
Point Group: C_s

Length: 12.86 Å
Width: 10.42 Å
Breadth: 3.890 Å
L/B Ratio: 1.234

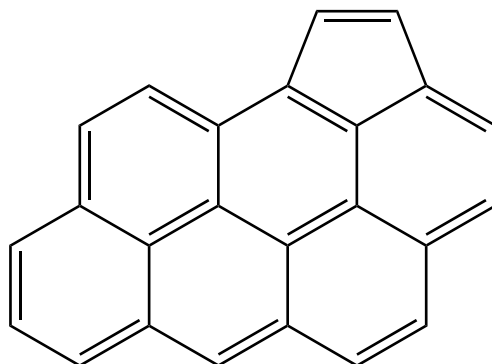
Cartesian coordinates:

C	4.6002	-0.5219	0.0000	C	0.9835	-0.2393	0.0000	H	5.5325	-1.0831	0.0000
C	4.4589	0.8353	0.0000	C	0.2034	0.9550	0.0000	H	5.2554	1.5766	0.0000
C	3.0258	1.1867	0.0000	C	-0.9933	-1.6754	0.0000	H	3.4152	-3.3156	0.0000
C	2.3517	-0.0848	0.0000	C	-3.7931	-1.8804	0.0000	H	0.9384	-3.6395	0.0000
C	3.2710	-1.1596	0.0000	C	-3.0086	-3.0156	0.0000	H	2.7297	3.3197	0.0000
C	2.7571	-2.4412	0.0000	C	-1.6125	-2.9166	0.0000	H	0.4657	4.3515	0.0000
C	1.3557	-2.6212	0.0000	C	-1.7924	-0.4959	0.0000	H	-1.9994	4.1376	0.0000
C	2.2768	2.3226	0.0000	C	-1.2070	0.8176	0.0000	H	-4.8860	-1.9620	0.0000
C	0.8334	2.2121	0.0000	C	-2.0010	1.9702	0.0000	H	-3.4757	-4.0061	0.0000
C	-0.0010	3.3596	0.0000	C	-3.4271	1.8234	0.0000	H	-0.9837	-3.8197	0.0000
C	-1.3692	3.2406	0.0000	C	-3.9956	0.5903	0.0000	H	-4.0438	2.7293	0.0000
C	0.4597	-1.5537	0.0000	C	-3.1967	-0.6040	0.0000	H	-5.0862	0.4782	0.0000

Table 3.159: Table of thermodynamic data as a function of temperature for Benzo[ghi]cyclopenta[cd]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-41.303	427.471	427.471	∞
100	85.428	318.427	677.708	-35.928	448.135	479.013	-250.206
200	179.835	404.952	519.479	-22.905	437.170	514.267	-134.310
250	234.335	450.900	501.136	-12.559	432.036	534.135	-111.599
298.15	287.164	496.705	496.705	0.000	427.471	554.225	-97.096
300	289.166	498.488	496.711	0.533	427.302	555.010	-96.634
350	341.723	547.052	500.426	16.319	423.090	576.637	-86.057
400	390.388	595.908	509.308	34.640	419.421	598.821	-78.196
450	434.435	644.479	521.633	55.280	416.224	621.442	-72.134
500	473.776	692.328	536.318	78.005	413.424	644.415	-67.320
600	539.632	784.770	570.090	128.808	408.781	691.071	-60.162
700	591.520	872.006	607.055	185.466	405.259	738.418	-55.100
800	632.932	953.796	645.342	246.764	402.735	786.187	-51.332
900	666.499	1030.350	683.914	311.792	401.079	834.213	-48.415
1000	694.084	1102.046	722.181	379.865	400.176	882.394	-46.091
1100	717.010	1169.307	759.804	450.454	399.875	930.643	-44.192
1200	736.240	1232.544	796.591	523.144	400.073	978.881	-42.609
1300	752.497	1292.134	832.440	597.603	400.630	1027.097	-41.268
1400	766.333	1348.420	867.304	673.563	401.446	1075.263	-40.118
1500	778.184	1401.706	901.170	750.804	402.463	1123.365	-39.118
1600	788.392	1452.263	934.047	829.145	403.578	1171.388	-38.241
1700	797.233	1500.330	965.956	908.436	404.738	1219.319	-37.464
1800	804.929	1546.122	996.926	988.553	405.882	1267.237	-36.773
1900	811.661	1589.826	1026.990	1069.390	406.991	1315.046	-36.152
2000	817.577	1631.613	1056.184	1150.858	408.024	1362.822	-35.593
2100	822.798	1671.632	1084.545	1232.882	408.916	1410.537	-35.084
2200	827.426	1710.017	1112.109	1315.398	409.669	1458.213	-34.622
2300	831.544	1746.890	1138.912	1398.351	410.284	1505.861	-34.198
2400	835.221	1782.360	1164.988	1481.692	410.700	1553.441	-33.809
2500	838.517	1816.523	1190.370	1565.382	410.929	1601.107	-33.453
2600	841.481	1849.469	1215.090	1649.385	410.944	1648.666	-33.121
2700	844.155	1881.278	1239.178	1733.669	410.748	1696.294	-32.816
2800	846.575	1912.022	1262.662	1818.207	410.320	1743.949	-32.533
2900	848.771	1941.768	1285.570	1902.976	409.637	1791.579	-32.269
3000	850.770	1970.577	1307.926	1987.955	408.738	1839.260	-32.024
3100	852.594	1998.504	1329.754	2073.124	407.556	1886.906	-31.793
3200	854.262	2025.600	1351.078	2158.469	406.128	1934.660	-31.579
3300	855.792	2051.910	1371.919	2243.972	404.440	1982.498	-31.380
3400	857.197	2077.480	1392.296	2329.623	402.466	2030.313	-31.191
3500	858.492	2102.347	1412.230	2415.408	400.213	2078.175	-31.014
3600	859.687	2126.548	1431.737	2501.318	397.701	2126.184	-30.849
3700	860.791	2150.118	1450.836	2587.342	394.902	2174.277	-30.695
3800	861.814	2173.087	1469.542	2673.473	391.795	2222.402	-30.548
3900	862.764	2195.486	1487.870	2759.703	388.414	2270.563	-30.410
4000	863.647	2217.340	1505.834	2846.024	384.747	2318.938	-30.282
4100	864.469	2238.676	1523.449	2932.430	380.763	2367.344	-30.160
4200	865.236	2259.517	1540.728	3018.916	376.487	2415.843	-30.045
4300	865.952	2279.885	1557.681	3105.476	371.907	2464.368	-29.936
4400	866.621	2299.801	1574.322	3192.105	367.030	2513.083	-29.833
4500	867.249	2319.283	1590.661	3278.799	361.870	2561.959	-29.738
4600	867.837	2338.351	1606.709	3365.553	356.380	2610.965	-29.648
4700	868.390	2357.021	1622.475	3452.365	350.576	2659.993	-29.562
4800	868.910	2375.309	1637.969	3539.230	344.495	2709.240	-29.482
4900	869.399	2393.230	1653.200	3626.146	338.075	2758.498	-29.405
5000	869.860	2410.799	1668.177	3713.109	331.396	2808.051	-29.335

3.160. Dibenzo[*def,mno*]cyclopenta[*hi*]chrysene



Formula: $C_{24}H_{12}$
Mass: 300.352 g/mol
CAS Number: 96915-19-4
Point Group: C_s

Length: 13.75 Å
Width: 10.48 Å
Breadth: 3.885 Å
L/B Ratio: 1.312

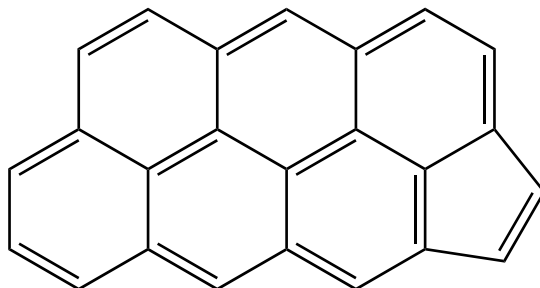
Cartesian coordinates:

C	2.0798	0.0940	0.0000	C	-1.9530	-3.0427	0.0000	H	-1.8777	3.9864	0.0000
C	2.5940	-1.2246	0.0000	C	-0.6147	-3.2444	0.0000	H	-4.3792	3.0347	0.0000
C	3.9949	-1.4084	0.0000	C	-2.0467	0.6506	0.0000	H	5.0291	1.8344	0.0000
C	4.8426	-0.3225	0.0000	C	-3.4251	0.9830	0.0000	H	5.9273	-0.4746	0.0000
C	4.3362	0.9852	0.0000	C	-4.3347	-0.0535	0.0000	H	4.3996	-2.4271	0.0000
C	2.9674	1.2046	0.0000	C	-3.8676	-1.3897	0.0000	H	2.1334	-3.3545	0.0000
C	0.6713	0.3082	0.0000	C	0.1418	1.6559	0.0000	H	-0.2084	-4.2629	0.0000
C	-0.1646	-0.8198	0.0000	C	-1.2258	1.8214	0.0000	H	-2.6500	-3.8882	0.0000
C	0.3476	-2.1548	0.0000	C	2.4123	2.5413	0.0000	H	-4.6038	-2.2016	0.0000
C	1.7086	-2.3433	0.0000	C	1.0798	2.7540	0.0000	H	-5.4119	0.1409	0.0000
C	-1.5716	-0.6457	0.0000	C	-2.1815	2.9412	0.0000	H	0.6662	3.7695	0.0000
C	-2.5124	-1.7067	0.0000	C	-3.4583	2.4554	0.0000	H	3.1161	3.3819	0.0000

Table 3.160: Table of thermodynamic data as a function of temperature for Dibenzo[def,mno]cyclopenta[hi]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-41.499	451.373	451.373	∞
100	85.653	318.351	679.657	-36.131	471.834	502.720	-262.589
200	180.969	405.343	520.519	-23.035	460.942	537.961	-140.498
250	235.682	451.570	502.075	-12.626	455.871	557.802	-116.544
298.15	288.583	497.621	497.621	0.000	451.373	577.854	-101.235
300	290.585	499.412	497.626	0.536	451.206	578.637	-100.748
350	343.125	548.194	501.359	16.392	447.065	600.212	-89.575
400	391.725	597.234	510.279	34.782	443.465	622.334	-81.267
450	435.686	645.958	522.653	55.487	440.332	644.885	-74.855
500	474.934	693.933	537.390	78.272	437.593	667.781	-69.761
600	540.615	786.571	571.268	129.182	433.056	714.266	-62.181
700	592.356	873.948	608.332	185.931	429.625	761.426	-56.817
800	633.650	955.841	646.709	247.306	427.179	808.995	-52.821
900	667.121	1032.473	685.361	312.401	425.590	856.812	-49.727
1000	694.629	1104.231	723.699	380.532	424.745	904.777	-47.260
1100	717.491	1171.541	761.385	451.172	424.495	952.806	-45.244
1200	736.667	1234.817	798.228	523.907	424.738	1000.818	-43.564
1300	752.878	1294.440	834.127	598.407	425.336	1048.805	-42.141
1400	766.675	1350.752	869.036	674.403	426.187	1096.739	-40.919
1500	778.492	1404.061	902.944	751.676	427.237	1144.607	-39.858
1600	788.671	1454.637	935.858	830.046	428.381	1192.393	-38.927
1700	797.487	1502.720	967.800	909.365	429.568	1240.086	-38.102
1800	805.161	1548.526	998.800	989.506	430.737	1287.764	-37.369
1900	811.874	1592.242	1028.892	1070.365	431.868	1335.333	-36.710
2000	817.772	1634.039	1058.112	1151.854	432.920	1382.866	-36.116
2100	822.978	1674.067	1086.497	1233.896	433.831	1430.338	-35.577
2200	827.592	1712.460	1114.083	1316.429	434.602	1477.771	-35.086
2300	831.697	1749.341	1140.907	1399.398	435.233	1525.173	-34.637
2400	835.364	1784.816	1167.002	1482.754	435.663	1572.509	-34.224
2500	838.650	1818.985	1192.402	1566.458	435.907	1619.928	-33.846
2600	841.605	1851.936	1217.139	1650.473	435.934	1667.241	-33.495
2700	844.271	1883.750	1241.243	1734.769	435.750	1714.622	-33.171
2800	846.684	1914.498	1264.741	1819.319	435.334	1762.029	-32.870
2900	848.873	1944.248	1287.662	1904.098	434.661	1809.412	-32.590
3000	850.866	1973.060	1310.031	1989.087	433.772	1856.845	-32.330
3100	852.684	2000.990	1331.872	2074.266	432.599	1904.242	-32.086
3200	854.347	2028.088	1353.208	2159.619	431.179	1951.747	-31.858
3300	855.872	2054.402	1374.059	2245.131	429.499	1999.336	-31.646
3400	857.273	2079.973	1394.447	2330.789	427.534	2046.902	-31.446
3500	858.564	2104.842	1414.390	2416.582	425.288	2094.514	-31.258
3600	859.755	2129.046	1433.907	2502.498	422.783	2142.274	-31.083
3700	860.856	2152.617	1453.015	2588.530	419.990	2190.117	-30.918
3800	861.876	2175.589	1471.729	2674.667	416.890	2237.992	-30.763
3900	862.823	2197.989	1490.065	2760.902	413.515	2285.903	-30.616
4000	863.703	2219.845	1508.037	2847.229	409.854	2334.027	-30.479
4100	864.522	2241.182	1525.660	2933.641	405.876	2382.182	-30.349
4200	865.286	2262.024	1542.945	3020.132	401.605	2430.431	-30.226
4300	866.000	2282.393	1559.906	3106.697	397.029	2478.706	-30.110
4400	866.668	2302.310	1576.553	3193.330	392.157	2527.170	-30.001
4500	867.294	2321.793	1592.898	3280.029	387.001	2575.795	-29.898
4600	867.880	2340.862	1608.952	3366.788	381.516	2624.550	-29.802
4700	868.431	2359.533	1624.724	3453.604	375.716	2673.326	-29.710
4800	868.949	2377.822	1640.223	3540.473	369.640	2722.322	-29.624
4900	869.437	2395.744	1655.460	3627.392	363.223	2771.328	-29.542
5000	869.897	2413.314	1670.442	3714.359	356.548	2820.630	-29.466

3.161. Benz[*mno*]indeno[1,7,6,5-*cdef*]chrysene



Formula: C₂₄H₁₂
Mass: 300.352 g/mol
CAS Number: 96915-21-8
Point Group: C_s

Length: 13.90 Å
Width: 9.572 Å
Breadth: 3.884 Å
L/B Ratio: 1.452

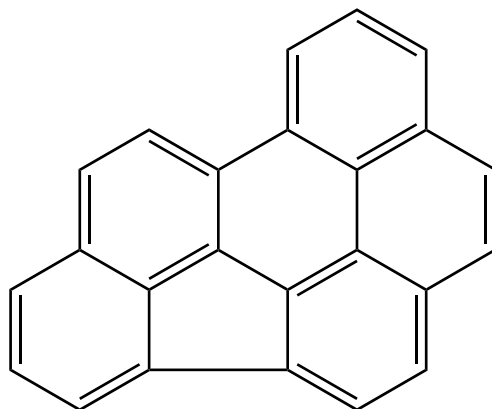
Cartesian coordinates:

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C	-4.0229	2.0857	0.0000	C	-1.4089	-0.4600	0.0000	H	5.6022	-0.5242	0.0000
C	-4.7586	0.9353	0.0000	C	-1.5273	-1.8649	0.0000	H	5.6768	1.9520	0.0000
C	-3.8557	-0.2291	0.0000	C	-0.3116	-2.6105	0.0000	H	3.5890	3.2867	0.0000
C	4.6656	0.0447	0.0000	C	-0.1735	0.2339	0.0000	H	1.1324	3.3985	0.0000
C	4.7046	1.4473	0.0000	C	0.9923	-0.5293	0.0000	H	-1.3606	3.5175	0.0000
C	3.5447	2.1917	0.0000	C	0.9079	-1.9654	0.0000	H	-4.9707	-2.0901	0.0000
C	2.2848	1.5527	0.0000	C	2.1600	-2.6961	0.0000	H	-2.9358	-3.5060	0.0000
C	1.0699	2.3031	0.0000	C	3.3517	-2.0630	0.0000	H	-0.3612	-3.7057	0.0000
C	-0.1534	1.6739	0.0000	C	3.4484	-0.6177	0.0000	H	2.1070	-3.7912	0.0000
C	-1.4104	2.4233	0.0000	C	2.2471	0.1394	0.0000	H	4.2895	-2.6307	0.0000

Table 3.161: Table of thermodynamic data as a function of temperature for Benz[*mno*]indeno[1,7,6,5-*cdef*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-41.286	454.182	454.182	∞
100	84.645	317.462	677.270	-35.981	474.793	505.768	-264.180
200	180.187	403.773	518.685	-22.982	463.803	541.137	-141.327
250	235.159	449.854	500.278	-12.606	458.700	561.060	-117.225
298.15	288.246	495.830	495.830	0.000	454.182	581.197	-101.821
300	290.254	497.619	495.835	0.535	454.015	581.983	-101.330
350	342.913	546.360	499.564	16.378	449.860	603.649	-90.088
400	391.580	595.376	508.478	34.759	446.251	625.864	-81.728
450	435.577	644.085	520.844	55.458	443.112	648.508	-75.275
500	474.845	692.051	535.574	78.238	440.368	671.497	-70.149
600	540.545	784.674	569.440	129.140	435.824	718.172	-62.521
700	592.299	872.041	606.494	185.883	432.386	765.521	-57.123
800	633.603	953.927	644.862	247.253	429.934	813.282	-53.101
900	667.086	1030.555	683.506	312.343	428.341	861.291	-49.987
1000	694.603	1102.309	721.838	380.472	427.493	909.448	-47.504
1100	717.473	1169.617	759.518	451.110	427.241	957.669	-45.475
1200	736.656	1232.892	796.356	523.843	427.483	1005.874	-43.784
1300	752.871	1292.514	832.251	598.342	428.080	1054.053	-42.352
1400	766.673	1348.826	867.157	674.337	428.931	1102.180	-41.122
1500	778.493	1402.134	901.061	751.611	429.980	1150.240	-40.054
1600	788.674	1452.710	933.972	829.981	431.125	1198.219	-39.117
1700	797.491	1500.794	965.912	909.300	432.312	1246.105	-38.287
1800	805.166	1546.600	996.910	989.442	433.481	1293.975	-37.549
1900	811.879	1590.317	1027.000	1070.301	434.613	1341.736	-36.886
2000	817.778	1632.114	1056.219	1151.790	435.666	1389.462	-36.288
2100	822.985	1672.142	1084.602	1233.834	436.577	1437.127	-35.746
2200	827.599	1710.536	1112.187	1316.367	437.349	1484.752	-35.252
2300	831.704	1747.416	1139.009	1399.337	437.980	1532.347	-34.800
2400	835.370	1782.892	1165.103	1482.694	438.411	1579.875	-34.384
2500	838.656	1817.062	1190.502	1566.398	438.655	1627.487	-34.004
2600	841.611	1850.013	1215.238	1650.414	438.683	1674.992	-33.650
2700	844.277	1881.826	1239.341	1734.710	438.500	1722.565	-33.324
2800	846.690	1912.575	1262.839	1819.261	438.084	1770.165	-33.022
2900	848.879	1942.325	1285.759	1904.041	437.413	1817.739	-32.740
3000	850.872	1971.138	1308.128	1989.030	436.524	1865.365	-32.478
3100	852.690	1999.068	1329.968	2074.209	435.351	1912.955	-32.232
3200	854.352	2026.166	1351.303	2159.563	433.932	1960.652	-32.004
3300	855.877	2052.480	1372.154	2245.075	432.253	2008.433	-31.790
3400	857.278	2078.051	1392.541	2330.734	430.288	2056.191	-31.589
3500	858.569	2102.920	1412.484	2416.527	428.043	2103.995	-31.400
3600	859.759	2127.124	1432.001	2502.444	425.538	2151.947	-31.223
3700	860.860	2150.696	1451.108	2588.476	422.746	2199.982	-31.058
3800	861.880	2173.667	1469.821	2674.614	419.645	2248.049	-30.901
3900	862.827	2196.067	1488.157	2760.850	416.271	2296.152	-30.753
4000	863.707	2217.923	1506.129	2847.177	412.611	2344.469	-30.615
4100	864.526	2239.261	1523.751	2933.589	408.633	2392.817	-30.484
4200	865.290	2260.103	1541.036	3020.080	404.362	2441.257	-30.361
4300	866.004	2280.472	1557.996	3106.645	399.787	2489.724	-30.244
4400	866.671	2300.389	1574.644	3193.280	394.915	2538.380	-30.134
4500	867.297	2319.873	1590.988	3279.978	389.760	2587.198	-30.031
4600	867.883	2338.941	1607.042	3366.738	384.275	2636.144	-29.934
4700	868.434	2357.612	1622.813	3453.554	378.475	2685.113	-29.841
4800	868.952	2375.901	1638.313	3540.423	372.399	2734.301	-29.755
4900	869.440	2393.823	1653.549	3627.343	365.983	2783.499	-29.672
5000	869.899	2411.393	1668.531	3714.310	359.308	2832.993	-29.595

3.162. Acenaphtho[1,2,3-*cde*]pyrene



Formula: C₂₄H₁₂
Mass: 300.352 g/mol
CAS Number: 75449-91-1
Point Group: C_s

Length: 13.35 Å
Width: 10.45 Å
Breadth: 3.885 Å
L/B Ratio: 1.278

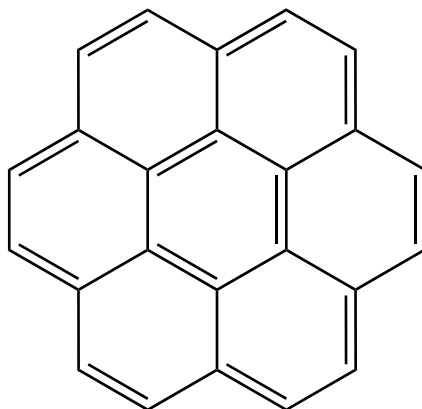
Cartesian coordinates:

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C	-0.1198	-0.8289	0.0000	C	1.8915	2.8837	0.0000	H	-0.8983	-4.1122	0.0000
C	-0.8347	0.4006	0.0000	C	1.2556	-0.8157	0.0000	H	3.8848	-2.9721	0.0000
C	-2.2003	0.0578	0.0000	C	1.8990	0.4686	0.0000	H	5.0824	-0.8098	0.0000
C	-2.3635	-1.3753	0.0000	C	1.1614	1.6990	0.0000	H	5.0903	1.6739	0.0000
C	1.0767	-3.2182	0.0000	C	-0.3056	1.6639	0.0000	H	3.8350	3.8093	0.0000
C	-0.3311	-3.1762	0.0000	C	-1.3083	2.6888	0.0000	H	1.3661	3.8458	0.0000
C	1.8928	-2.0717	0.0000	C	-2.6586	2.3905	0.0000	H	-0.9869	3.7365	0.0000
C	3.3334	-2.0256	0.0000	C	-3.1665	1.0468	0.0000	H	-3.3882	3.2081	0.0000
C	3.9859	-0.8337	0.0000	C	-4.4969	0.5373	0.0000	H	-5.3427	1.2323	0.0000
C	3.3064	0.4455	0.0000	C	-4.7026	-0.8255	0.0000	H	-5.7332	-1.1992	0.0000
C	3.9946	1.6672	0.0000	C	-3.6614	-1.8059	0.0000	H	-3.9244	-2.8679	0.0000

Table 3.162: Table of thermodynamic data as a function of temperature for Acenaphtho[1,2,3-*cde*]pyrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-41.181	458.615	458.615	∞
100	85.396	319.244	677.123	-35.788	479.419	510.216	-266.504
200	179.032	405.482	519.538	-22.811	468.408	545.399	-142.441
250	233.356	451.229	501.269	-12.510	463.229	565.246	-118.099
298.15	286.115	496.855	496.855	0.000	458.615	585.324	-102.544
300	288.115	498.631	496.861	0.531	458.444	586.109	-102.048
350	340.663	547.032	500.563	16.264	454.179	607.733	-90.697
400	389.352	595.748	509.417	34.533	450.458	629.922	-82.258
450	433.444	644.199	521.705	55.122	447.209	652.554	-75.745
500	472.841	691.947	536.349	77.799	444.362	675.543	-70.572
600	538.830	784.230	570.039	128.514	439.631	722.246	-62.876
700	590.858	871.353	606.925	185.100	436.037	769.653	-57.431
800	632.401	953.064	645.141	246.338	433.453	817.491	-53.376
900	666.081	1029.561	683.652	311.319	431.750	865.594	-50.237
1000	693.759	1101.218	721.864	379.354	430.809	913.855	-47.734
1100	716.759	1168.452	759.439	449.915	430.480	962.189	-45.690
1200	736.048	1231.669	796.184	522.583	430.656	1010.513	-43.986
1300	752.349	1291.246	831.996	597.025	431.196	1058.817	-42.543
1400	766.221	1347.523	866.828	672.972	431.999	1107.072	-41.305
1500	778.099	1400.802	900.667	750.203	433.006	1155.265	-40.229
1600	788.328	1451.354	933.518	828.537	434.114	1203.378	-39.285
1700	797.186	1499.418	965.405	907.823	435.268	1251.401	-38.450
1800	804.894	1545.207	996.354	987.936	436.409	1299.410	-37.707
1900	811.636	1588.910	1026.400	1068.769	437.514	1347.310	-37.039
2000	817.560	1630.695	1055.578	1150.236	438.545	1395.178	-36.438
2100	822.787	1670.713	1083.924	1232.258	439.435	1442.985	-35.892
2200	827.419	1709.098	1111.474	1314.773	440.188	1490.753	-35.394
2300	831.540	1745.971	1138.265	1397.725	440.802	1538.492	-34.940
2400	835.220	1781.441	1164.330	1481.067	441.218	1586.165	-34.521
2500	838.519	1815.604	1189.701	1564.756	441.447	1633.922	-34.138
2600	841.484	1848.550	1214.412	1648.759	441.462	1681.573	-33.783
2700	844.160	1880.359	1238.491	1733.044	441.267	1729.293	-33.455
2800	846.581	1911.104	1261.967	1817.583	440.840	1777.040	-33.150
2900	848.778	1940.850	1284.867	1902.352	440.157	1824.762	-32.867
3000	850.777	1969.659	1307.215	1987.332	439.259	1872.535	-32.603
3100	852.601	1997.586	1329.037	2072.502	438.077	1920.273	-32.356
3200	854.270	2024.682	1350.355	2157.847	436.650	1968.118	-32.126
3300	855.800	2050.993	1371.190	2243.351	434.962	2016.048	-31.911
3400	857.205	2076.562	1391.562	2329.003	432.990	2063.954	-31.708
3500	858.500	2101.430	1411.490	2414.789	430.738	2111.908	-31.518
3600	859.695	2125.631	1430.993	2500.699	428.226	2160.009	-31.340
3700	860.799	2149.201	1450.087	2586.725	425.428	2208.194	-31.173
3800	861.822	2172.171	1468.788	2672.856	422.321	2256.410	-31.016
3900	862.772	2194.570	1487.112	2759.087	418.942	2304.663	-30.867
4000	863.654	2216.425	1505.072	2845.409	415.276	2353.129	-30.728
4100	864.476	2237.761	1522.684	2931.816	411.293	2401.627	-30.596
4200	865.243	2258.602	1539.958	3018.302	407.017	2450.217	-30.472
4300	865.959	2278.970	1556.909	3104.862	402.437	2498.834	-30.354
4400	866.629	2298.886	1573.546	3191.492	397.561	2547.641	-30.244
4500	867.256	2318.368	1589.882	3278.187	392.402	2596.609	-30.140
4600	867.844	2337.436	1605.927	3364.942	386.913	2645.706	-30.042
4700	868.397	2356.106	1621.690	3451.754	381.109	2694.825	-29.949
4800	868.916	2374.394	1637.182	3538.620	375.029	2744.164	-29.862
4900	869.405	2392.316	1652.410	3625.537	368.610	2793.513	-29.779
5000	869.866	2409.885	1667.385	3712.500	361.931	2843.157	-29.702

3.163. Coronene



Other names: Dibenzo[*ghi,pqr*]perylene
Hexabenzobenzene

Formula: $C_{24}H_{12}$
Mass: 300.352 g/mol
CAS Number: 191-07-1
Point Group: D_{6h}

Length: 11.64 Å
Width: 11.63 Å
Breadth: 3.888 Å
L/B Ratio: 1.000

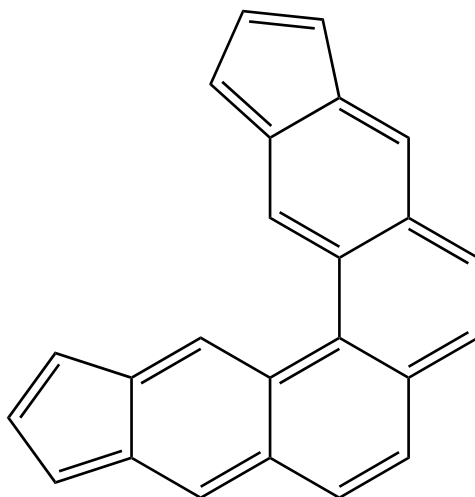
Cartesian coordinates:

C	-3.7358	-0.0276	0.0000	C	3.4963	-1.3164	0.0000	H	-4.7624	-0.4116	0.0000
C	-3.4963	1.3165	0.0000	C	3.7358	0.0277	0.0000	H	-4.3270	2.0314	0.0000
C	-2.1636	1.8222	0.0000	C	2.1637	-1.8222	0.0000	H	-0.4043	4.7630	0.0000
C	-1.0918	0.9195	0.0000	C	1.0918	-0.9196	0.0000	H	-2.7377	3.9185	0.0000
C	-0.6081	3.6861	0.0000	C	0.6081	-3.6861	0.0000	H	3.9227	2.7317	0.0000
C	-1.8918	3.2215	0.0000	C	1.8919	-3.2215	0.0000	H	2.0246	4.3301	0.0000
C	0.4962	2.7848	0.0000	C	-0.4963	-2.7849	0.0000	H	4.3270	-2.0313	0.0000
C	0.2504	1.4053	0.0000	C	-0.2504	-1.4053	0.0000	H	4.7624	0.4117	0.0000
C	2.8882	2.3697	0.0000	C	-1.3423	-0.4858	0.0000	H	0.4043	-4.7630	0.0000
C	1.8439	3.2491	0.0000	C	-2.6599	-0.9627	0.0000	H	2.7377	-3.9185	0.0000
C	2.6599	0.9627	0.0000	C	-2.8882	-2.3697	0.0000	H	-3.9228	-2.7316	0.0000
C	1.3423	0.4858	0.0000	C	-1.8440	-3.2492	0.0000	H	-2.0246	-4.3302	0.0000

Table 3.163: Table of thermodynamic data as a function of temperature for Coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-40.585	306.608	306.608	∞
100	81.865	293.505	647.680	-35.417	316.075	349.445	-182.528
200	177.490	377.911	491.374	-22.693	304.811	387.317	-101.155
250	232.200	423.364	473.192	-12.457	299.567	408.550	-85.360
298.15	285.041	468.796	468.796	0.000	294.900	429.975	-75.328
300	287.041	470.565	468.801	0.529	294.727	430.812	-75.009
350	339.585	518.800	472.491	16.208	290.408	453.844	-67.731
400	388.280	567.373	481.315	34.423	286.633	477.447	-62.347
450	432.408	615.700	493.566	54.960	283.332	501.501	-58.212
500	471.869	663.341	508.169	77.586	280.434	525.919	-54.941
600	538.019	755.461	541.773	128.213	275.615	575.490	-50.100
700	590.209	842.471	578.579	184.725	271.947	625.780	-46.695
800	631.889	924.104	616.723	245.905	269.305	676.511	-44.171
900	665.678	1000.548	655.170	310.840	267.556	727.512	-42.223
1000	693.441	1072.168	693.327	378.840	266.580	778.677	-40.673
1100	716.507	1139.374	730.854	449.372	266.222	829.917	-39.409
1200	735.846	1202.572	767.557	522.018	266.376	881.150	-38.355
1300	752.186	1262.134	803.333	596.442	266.898	932.365	-37.462
1400	766.088	1318.400	838.133	672.374	267.686	983.532	-36.695
1500	777.989	1371.670	871.942	749.593	268.681	1034.637	-36.029
1600	788.237	1422.216	904.768	827.917	269.779	1085.664	-35.443
1700	797.109	1470.275	936.631	907.194	270.924	1136.600	-34.923
1800	804.829	1516.060	967.560	987.300	272.058	1187.524	-34.460
1900	811.581	1559.760	997.587	1068.128	273.158	1238.339	-34.044
2000	817.512	1601.543	1026.748	1149.589	274.183	1289.122	-33.668
2100	822.746	1641.558	1055.079	1231.607	275.069	1339.844	-33.326
2200	827.383	1679.942	1082.615	1314.118	275.818	1390.528	-33.015
2300	831.509	1716.813	1109.393	1397.067	276.429	1441.183	-32.730
2400	835.193	1752.281	1135.446	1480.405	276.841	1491.772	-32.467
2500	838.494	1786.443	1160.806	1564.093	277.069	1542.445	-32.227
2600	841.462	1819.389	1185.507	1648.093	277.081	1593.012	-32.003
2700	844.140	1851.197	1209.576	1732.375	276.883	1643.648	-31.798
2800	846.563	1881.941	1233.043	1816.913	276.455	1694.311	-31.607
2900	848.762	1911.687	1255.935	1901.681	275.771	1744.949	-31.429
3000	850.763	1940.495	1278.276	1986.658	274.870	1795.639	-31.264
3100	852.588	1968.422	1300.090	2071.827	273.687	1846.293	-31.109
3200	854.258	1995.517	1321.401	2157.171	272.259	1897.055	-30.966
3300	855.789	2021.828	1342.230	2242.674	270.570	1947.901	-30.832
3400	857.195	2047.397	1362.596	2328.324	268.596	1998.724	-30.706
3500	858.491	2072.264	1382.518	2414.110	266.344	2049.594	-30.588
3600	859.686	2096.465	1402.015	2500.019	263.831	2100.612	-30.478
3700	860.791	2120.035	1421.104	2586.044	261.032	2151.713	-30.376
3800	861.815	2143.004	1439.801	2672.175	257.925	2202.846	-30.280
3900	862.765	2165.403	1458.120	2758.404	254.544	2254.016	-30.189
4000	863.648	2187.258	1476.076	2844.725	250.877	2305.399	-30.105
4100	864.470	2208.594	1493.683	2931.132	246.894	2356.813	-30.026
4200	865.237	2229.434	1510.954	3017.618	242.618	2408.321	-29.951
4300	865.953	2249.802	1527.901	3104.177	238.037	2459.854	-29.881
4400	866.623	2269.718	1544.535	3190.807	233.161	2511.578	-29.816
4500	867.251	2289.201	1560.867	3277.501	228.001	2563.462	-29.755
4600	867.840	2308.268	1576.908	3364.256	222.512	2615.476	-29.699
4700	868.392	2326.938	1592.669	3451.067	216.707	2667.512	-29.645
4800	868.912	2345.226	1608.157	3537.933	210.627	2719.767	-29.596
4900	869.402	2363.148	1623.383	3624.849	204.207	2772.033	-29.550
5000	869.863	2380.717	1638.354	3711.812	197.528	2824.594	-29.508

3.164. Cyclopent[*b*]indeno[4,5-*g*]phenanthrene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 72088-81-4
Point Group: C₂

Length: 14.31 Å
Width: 10.51 Å
Breadth: 5.138 Å
L/B Ratio: 1.362

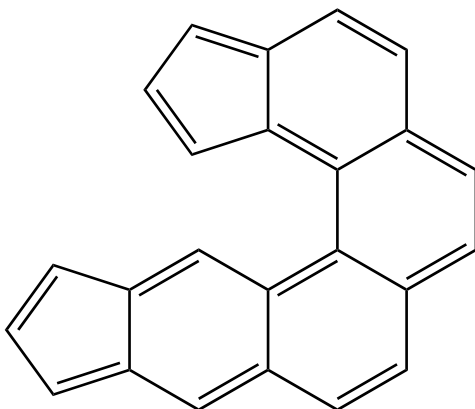
Cartesian coordinates:

C	4.9669	1.6101	-0.2077	C	-1.2222	-3.3390	0.4112	H	-5.9739	1.3196	0.0669
C	3.8294	0.6877	-0.2054	C	-2.4021	-2.7035	0.4938	H	5.1626	3.6664	0.5417
C	2.7129	1.4198	0.4159	C	-2.5017	-1.2773	0.2527	H	5.9471	1.3663	-0.6106
C	3.1593	2.6650	0.7694	C	-1.2707	-0.5190	0.0298	H	2.5958	3.4601	1.2526
C	4.5634	2.7733	0.3767	C	-1.4131	0.8960	-0.2689	H	4.5063	-1.1490	-1.0693
C	1.4337	0.7926	0.5114	C	-2.6292	1.4722	-0.2770	H	0.6058	1.3769	0.9363
C	1.2537	-0.4843	0.0551	C	-3.8536	0.7078	0.0034	H	3.1993	-3.1926	-0.8655
C	2.4106	-1.2534	-0.3983	C	-3.7337	-0.6896	0.2614	H	-1.1435	-4.4208	0.5690
C	3.6853	-0.5857	-0.6111	C	-3.0619	2.8472	-0.5375	H	-3.3234	-3.2481	0.7324
C	-0.0450	-1.1551	0.0725	C	-4.4188	2.8895	-0.4115	H	-4.6430	-1.2697	0.4571
C	-0.0089	-2.6118	0.0993	C	-4.9230	1.5591	-0.0777	H	-0.5170	1.4893	-0.4997
C	1.1283	-3.2975	-0.2170	H	-5.0609	3.7591	-0.5352	H	1.1325	-4.3937	-0.2358
C	2.3316	-2.6079	-0.5372	H	-2.3855	3.6632	-0.7804				

Table 3.164: Table of thermodynamic data as a function of temperature for Cyclopent[*b*]indeno[4,5-*g*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.105	693.127	693.127	∞
100	101.126	332.724	730.535	-39.781	715.406	754.927	-394.325
200	198.861	431.121	556.262	-25.028	703.477	799.223	-208.731
250	255.980	481.586	536.256	-13.667	697.961	823.799	-172.120
298.15	311.537	531.438	531.438	0.000	693.127	848.487	-148.648
300	313.640	533.372	531.444	0.578	692.950	849.450	-147.899
350	368.742	585.905	535.467	17.653	688.578	875.890	-130.717
400	419.485	638.511	545.062	37.379	684.857	902.902	-117.905
450	465.150	690.606	558.347	59.517	681.695	930.352	-107.990
500	505.732	741.758	574.140	83.809	679.002	958.146	-100.095
600	573.329	840.192	610.357	137.901	674.719	1014.402	-88.310
700	626.457	932.720	649.872	197.994	671.693	1071.277	-79.938
800	668.926	1019.245	690.697	262.839	669.763	1128.495	-73.682
900	703.491	1100.096	731.744	331.516	668.783	1185.892	-68.826
1000	732.045	1175.740	772.403	403.337	668.624	1243.364	-64.945
1100	755.903	1246.664	812.328	477.769	669.127	1300.827	-61.770
1200	776.017	1313.322	851.328	554.393	670.181	1358.203	-59.120
1300	793.100	1376.130	889.305	632.872	671.636	1415.484	-56.874
1400	807.699	1435.453	926.217	712.930	673.387	1472.644	-54.944
1500	820.247	1491.617	962.055	794.343	675.368	1529.674	-53.267
1600	831.089	1544.909	996.832	876.923	677.471	1586.557	-51.795
1700	840.505	1595.583	1030.575	960.514	679.635	1643.286	-50.491
1800	848.720	1643.862	1063.316	1044.984	681.800	1699.944	-49.330
1900	855.921	1689.947	1095.093	1130.224	683.939	1756.436	-48.287
2000	862.259	1734.015	1125.945	1216.139	686.009	1812.839	-47.346
2100	867.863	1776.223	1155.913	1302.651	687.943	1869.130	-46.491
2200	872.836	1816.713	1185.035	1389.691	689.742	1925.334	-45.712
2300	877.265	1855.612	1213.351	1477.200	691.402	1981.459	-44.999
2400	881.226	1893.033	1240.896	1565.128	692.863	2037.473	-44.344
2500	884.779	1929.080	1267.707	1653.432	694.137	2093.530	-43.741
2600	887.978	1963.845	1293.817	1742.072	695.191	2149.437	-43.182
2700	890.865	1997.412	1319.258	1831.017	696.032	2205.371	-42.665
2800	893.480	2029.859	1344.060	1920.236	696.636	2261.298	-42.184
2900	895.855	2061.255	1368.253	2009.705	696.979	2317.161	-41.736
3000	898.017	2091.662	1391.862	2099.400	697.099	2373.039	-41.317
3100	899.991	2121.141	1414.914	2189.302	696.929	2428.850	-40.925
3200	901.797	2149.743	1437.433	2279.393	696.506	2484.735	-40.558
3300	903.454	2177.519	1459.441	2369.657	695.813	2540.672	-40.215
3400	904.978	2204.513	1480.960	2460.079	694.828	2596.558	-39.890
3500	906.381	2230.766	1502.010	2550.648	693.554	2652.461	-39.585
3600	907.676	2256.318	1522.609	2641.352	692.011	2708.482	-39.298
3700	908.875	2281.204	1542.777	2732.180	690.171	2764.564	-39.028
3800	909.985	2305.457	1562.530	2823.124	688.012	2820.647	-38.772
3900	911.016	2329.108	1581.884	2914.174	685.569	2876.745	-38.529
4000	911.974	2352.185	1600.854	3005.325	682.829	2933.033	-38.301
4100	912.867	2374.715	1619.455	3096.567	679.761	2989.327	-38.084
4200	913.699	2396.723	1637.700	3187.896	676.389	3045.692	-37.878
4300	914.477	2418.232	1655.603	3279.305	672.700	3102.061	-37.682
4400	915.205	2439.264	1673.175	3370.790	668.703	3158.602	-37.497
4500	915.887	2459.839	1690.429	3462.345	664.411	3215.286	-37.321
4600	916.526	2479.976	1707.375	3553.966	659.778	3272.076	-37.155
4700	917.127	2499.694	1724.024	3645.649	654.817	3328.869	-36.995
4800	917.692	2519.008	1740.386	3737.390	649.569	3385.865	-36.845
4900	918.224	2537.936	1756.470	3829.186	643.970	3442.854	-36.701
5000	918.726	2556.492	1772.285	3921.034	638.100	3500.126	-36.565

3.165. Cyclopent[*b*]indeno[5,6-*g*]phenanthrene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 72088-82-5
Point Group: C₁

Length: 12.83 Å
Width: 10.69 Å
Breadth: 5.186 Å
L/B Ratio: 1.200

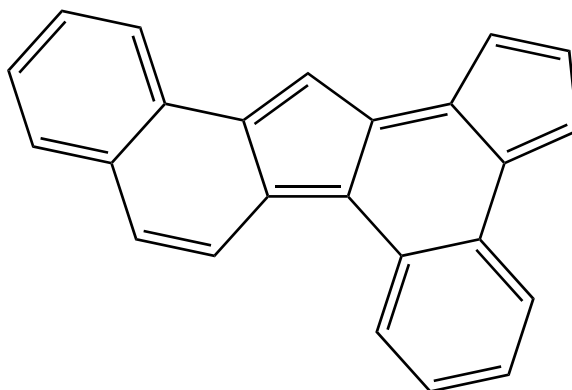
Cartesian coordinates:

C	-3.3847	-2.2747	-0.1779	C	0.5349	0.8659	-0.0737	H	2.9300	-2.8276	-0.1245
C	-1.9971	-2.4122	-0.0184	C	2.8411	1.7607	0.0077	H	1.1773	-3.5738	-0.0735
C	-1.2450	-1.2668	0.2244	C	3.3363	0.5122	-0.0252	H	0.4730	-1.5262	1.4950
C	-1.7716	0.0119	0.1154	C	2.4788	-0.6832	-0.1399	H	-1.3266	-4.5394	-0.3779
C	-3.1602	0.1608	-0.0095	C	1.0245	-0.5435	-0.3638	H	3.4900	2.6409	0.0814
C	-3.9501	-1.0077	-0.1321	C	3.2675	-1.7888	-0.0787	H	0.8548	-0.6980	-1.4619
C	-3.6642	1.5071	-0.0194	C	4.6616	-1.3525	0.0602	H	1.5678	4.1128	0.1170
C	-2.8177	2.5703	0.0495	C	4.7103	0.0065	0.0805	H	-0.8784	4.5196	0.1146
C	-1.3865	2.4091	0.0723	C	-1.0337	-3.5154	-0.1528	H	-3.2118	3.5930	0.0687
C	-0.8567	1.1137	0.0522	C	0.2264	-3.0395	0.0094	H	-4.7486	1.6542	-0.0741
C	-0.4853	3.4974	0.0862	C	0.2031	-1.5787	0.4113	H	-5.0363	-0.8955	-0.2242
C	0.8705	3.2677	0.0743	H	5.4987	-2.0435	0.1299	H	-4.0094	-3.1582	-0.3412
C	1.3992	1.9559	-0.0099	H	5.5853	0.6460	0.1697				

Table 3.165: Table of thermodynamic data as a function of temperature for Cyclopent[*b*]indeno[5,6-*g*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-43.684	738.063	738.063	∞
100	92.754	326.920	705.731	-37.881	762.241	802.343	-419.092
200	189.188	419.109	539.264	-24.031	749.410	847.558	-221.355
250	245.749	467.350	520.026	-13.169	743.396	872.792	-182.356
298.15	301.130	515.380	515.380	0.000	738.063	898.211	-157.360
300	303.234	517.249	515.386	0.559	737.867	899.203	-156.562
350	358.547	568.189	519.282	17.118	732.978	926.491	-138.268
400	409.775	619.463	528.600	36.345	728.759	954.423	-124.632
450	456.085	670.451	541.534	58.013	725.127	982.854	-114.084
500	497.391	720.685	556.945	81.870	721.999	1011.680	-105.687
600	566.469	817.730	592.393	135.202	716.956	1070.117	-93.160
700	620.947	909.304	631.193	194.678	713.313	1129.288	-84.267
800	664.556	995.170	671.382	259.030	710.891	1188.883	-77.624
900	700.042	1075.562	711.874	327.319	709.522	1248.711	-72.472
1000	729.323	1150.882	752.049	398.833	709.055	1308.654	-68.356
1100	753.749	1221.573	791.553	473.022	709.316	1368.615	-64.989
1200	774.303	1288.064	830.186	549.454	710.177	1428.509	-62.180
1300	791.727	1350.749	867.842	627.779	711.479	1488.322	-59.800
1400	806.591	1409.980	904.470	707.714	713.106	1548.026	-57.756
1500	819.347	1466.075	940.057	789.027	714.987	1607.606	-55.981
1600	830.352	1519.314	974.611	871.525	717.009	1667.046	-54.422
1700	839.896	1569.947	1008.154	955.048	719.106	1726.337	-53.043
1800	848.215	1618.195	1040.716	1039.463	721.215	1785.560	-51.815
1900	855.498	1664.255	1072.331	1124.657	723.309	1844.620	-50.711
2000	861.903	1708.303	1103.036	1210.534	725.339	1903.593	-49.716
2100	867.561	1750.495	1132.870	1297.013	727.240	1962.456	-48.812
2200	872.578	1790.972	1161.870	1384.024	729.011	2021.234	-47.989
2300	877.044	1829.860	1190.073	1471.510	730.647	2079.933	-47.236
2400	881.035	1867.273	1217.515	1559.417	732.088	2138.523	-46.543
2500	884.614	1903.312	1244.231	1647.703	733.344	2197.156	-45.906
2600	887.833	1938.071	1270.253	1736.328	734.383	2255.640	-45.315
2700	890.739	1971.634	1295.612	1825.259	735.210	2314.152	-44.769
2800	893.369	2004.076	1320.338	1914.467	735.803	2372.657	-44.262
2900	895.757	2035.468	1344.459	2003.925	736.135	2431.098	-43.788
3000	897.930	2065.873	1368.002	2093.611	736.246	2489.555	-43.346
3100	899.914	2095.348	1390.992	2183.505	736.067	2547.945	-42.932
3200	901.728	2123.949	1413.452	2273.588	735.637	2606.409	-42.544
3300	903.392	2151.722	1435.405	2363.845	734.938	2664.926	-42.181
3400	904.922	2178.714	1456.872	2454.262	733.947	2723.392	-41.839
3500	906.331	2204.966	1477.873	2544.826	732.667	2781.875	-41.516
3600	907.631	2230.517	1498.426	2635.525	731.119	2840.476	-41.213
3700	908.833	2255.401	1518.550	2726.349	729.275	2899.139	-40.928
3800	909.947	2279.653	1538.262	2817.288	727.112	2957.802	-40.657
3900	910.981	2303.303	1557.576	2908.336	724.666	3016.481	-40.400
4000	911.943	2326.380	1576.509	2999.482	721.923	3075.349	-40.159
4100	912.838	2348.909	1595.074	3090.722	718.852	3134.223	-39.930
4200	913.673	2370.916	1613.286	3182.048	715.477	3193.169	-39.712
4300	914.453	2392.425	1631.156	3273.455	711.785	3252.119	-39.505
4400	915.183	2413.456	1648.698	3364.937	707.786	3311.240	-39.309
4500	915.866	2434.030	1665.922	3456.490	703.492	3370.505	-39.123
4600	916.507	2454.167	1682.839	3548.109	698.857	3429.876	-38.947
4700	917.109	2473.884	1699.461	3639.790	693.894	3489.250	-38.778
4800	917.676	2493.199	1715.797	3731.529	688.645	3548.827	-38.618
4900	918.209	2512.126	1731.856	3823.324	683.043	3608.397	-38.465
5000	918.711	2530.681	1747.647	3915.170	677.173	3668.250	-38.321

3.166. Dibenzo[*c,i*]cyclopenta[*a*]fluorene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 63218-07-5
Point Group: C_s

Length: 14.83 Å
Width: 10.92 Å
Breadth: 3.885 Å
L/B Ratio: 1.358

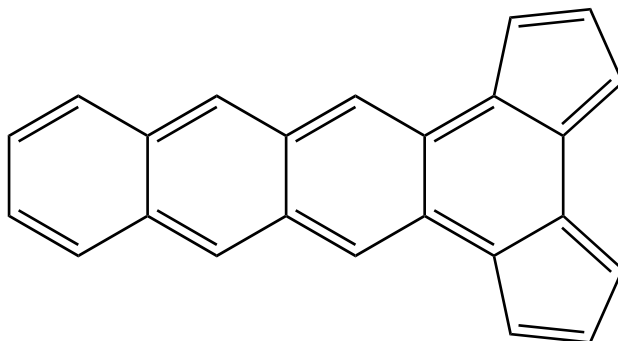
Cartesian coordinates:

C	-5.0558	-0.9169	0.0000	C	1.8493	1.7988	0.0000	H	5.2382	1.6307	0.0000
C	-3.6336	-0.8503	0.0000	C	3.0691	0.9731	0.0000	H	-5.5375	-1.9013	0.0000
C	-3.0070	0.4197	0.0000	C	3.0325	-0.3864	0.0000	H	-6.8967	0.1787	0.0000
C	-3.8101	1.5938	0.0000	C	1.7396	-1.0806	0.0000	H	-5.7959	2.3973	0.0000
C	-5.1733	1.4966	0.0000	C	1.7677	-2.5294	0.0000	H	-3.3152	2.5718	0.0000
C	-5.8029	0.2276	0.0000	C	2.9284	-3.2163	0.0000	H	-0.8833	-2.9044	0.0000
C	-2.8506	-2.0321	0.0000	C	4.1943	-2.5301	0.0000	H	-3.3631	-3.0011	0.0000
C	-1.4758	-1.9801	0.0000	C	4.2432	-1.1826	0.0000	H	-1.0079	2.6417	0.0000
C	-0.8390	-0.7305	0.0000	C	4.1902	1.9235	0.0000	H	5.2007	-0.6478	0.0000
C	-1.5970	0.4529	0.0000	C	3.6774	3.1827	0.0000	H	5.1093	-3.1315	0.0000
C	0.5854	-0.3542	0.0000	C	2.2102	3.1146	0.0000	H	0.8056	-3.0608	0.0000
C	0.5900	1.1257	0.0000	H	1.5574	3.9845	0.0000	H	2.9361	-4.3115	0.0000
C	-0.6876	1.6009	0.0000	H	4.2311	4.1191	0.0000				

Table 3.166: Table of thermodynamic data as a function of temperature for Dibenzoc[*c,i*]cyclopenta[*a*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.730	648.829	648.829	∞
100	105.318	345.274	746.399	-40.112	670.776	709.043	-370.358
200	200.469	445.857	571.154	-25.059	659.147	751.946	-196.384
250	256.232	496.531	551.143	-13.653	653.678	775.779	-162.087
298.15	310.734	546.333	546.333	0.000	648.829	799.748	-140.110
300	312.802	548.262	546.339	0.577	648.651	800.684	-139.409
350	367.118	600.603	550.349	17.589	644.216	826.384	-123.328
400	417.340	652.955	559.905	37.220	640.400	852.667	-111.345
450	462.693	704.778	573.130	59.241	637.122	879.401	-102.076
500	503.117	755.662	588.848	83.407	634.301	906.494	-94.699
600	570.681	853.612	624.890	137.233	629.753	961.384	-83.694
700	623.965	945.741	664.216	197.068	626.469	1016.938	-75.883
800	666.654	1031.948	704.855	261.674	624.301	1072.870	-70.050
900	701.448	1112.544	745.727	330.136	623.105	1129.010	-65.525
1000	730.216	1187.985	786.221	401.763	622.752	1185.248	-61.910
1100	754.268	1258.743	825.995	476.022	623.082	1241.495	-58.952
1200	774.554	1325.267	864.857	552.492	623.981	1297.670	-56.485
1300	791.786	1387.963	902.708	630.832	625.298	1353.762	-54.394
1400	806.516	1447.194	939.504	710.766	626.924	1409.744	-52.597
1500	819.179	1503.280	975.236	792.066	628.793	1465.603	-51.036
1600	830.121	1556.507	1009.917	874.544	630.794	1521.324	-49.665
1700	839.625	1607.124	1043.570	958.042	632.866	1576.896	-48.451
1800	847.917	1655.356	1076.229	1042.429	634.946	1632.402	-47.370
1900	855.186	1701.399	1107.930	1127.592	637.009	1687.747	-46.398
2000	861.585	1745.431	1138.712	1213.437	639.009	1743.007	-45.522
2100	867.242	1787.607	1168.615	1299.884	640.878	1798.157	-44.726
2200	872.262	1828.070	1197.677	1386.864	642.617	1853.225	-44.000
2300	876.735	1866.944	1225.936	1474.318	644.222	1908.215	-43.336
2400	880.734	1904.343	1253.429	1562.195	645.632	1963.097	-42.725
2500	884.322	1940.371	1280.190	1650.451	646.858	2018.024	-42.163
2600	887.551	1975.119	1306.254	1739.048	647.868	2072.802	-41.642
2700	890.467	2008.671	1331.652	1827.951	648.668	2127.610	-41.160
2800	893.107	2041.103	1356.413	1917.132	649.234	2182.412	-40.713
2900	895.505	2072.486	1380.567	2006.564	649.540	2237.151	-40.295
3000	897.688	2102.882	1404.141	2096.226	649.626	2291.906	-39.905
3100	899.682	2132.350	1427.158	2186.096	649.424	2346.596	-39.539
3200	901.506	2160.943	1449.645	2276.156	648.971	2401.360	-39.197
3300	903.179	2188.710	1471.622	2366.392	648.251	2456.178	-38.877
3400	904.717	2215.696	1493.111	2456.788	647.238	2510.945	-38.575
3500	906.134	2241.942	1514.133	2547.331	645.939	2565.730	-38.291
3600	907.443	2267.487	1534.707	2638.011	644.372	2620.634	-38.024
3700	908.653	2292.367	1554.849	2728.816	642.509	2675.600	-37.772
3800	909.774	2316.614	1574.578	2819.738	640.328	2730.566	-37.533
3900	910.815	2340.260	1593.909	2910.769	637.865	2785.549	-37.307
4000	911.783	2363.332	1612.857	3001.899	635.106	2840.722	-37.095
4100	912.684	2385.857	1631.437	3093.123	632.019	2895.902	-36.893
4200	913.525	2407.861	1649.663	3184.434	628.629	2951.153	-36.702
4300	914.310	2429.366	1667.546	3275.826	624.923	3006.409	-36.520
4400	915.045	2450.394	1685.100	3367.294	620.910	3061.836	-36.348
4500	915.734	2470.966	1702.336	3458.833	616.602	3117.407	-36.185
4600	916.380	2491.100	1719.265	3550.440	611.954	3173.084	-36.031
4700	916.987	2510.814	1735.897	3642.108	606.979	3228.766	-35.883
4800	917.557	2530.126	1752.243	3733.836	601.717	3284.650	-35.744
4900	918.095	2549.051	1768.312	3825.619	596.104	3340.527	-35.610
5000	918.601	2567.604	1784.113	3917.454	590.222	3396.688	-35.484

3.167. Dicyclopenta[*a,c*]naphthacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 15209-78-6
Point Group: C_{2v}

Length: 15.53 Å
Width: 10.10 Å
Breadth: 3.886 Å
L/B Ratio: 1.539

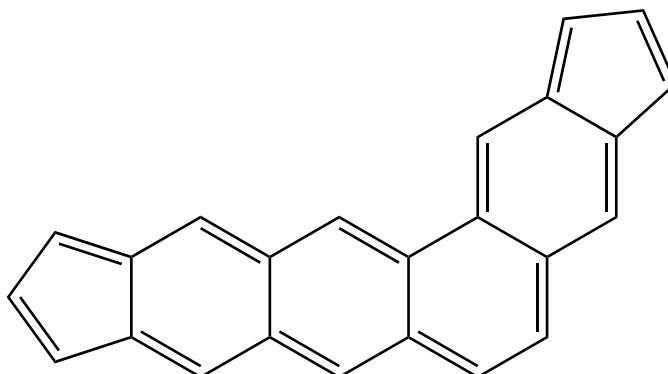
Cartesian coordinates:

C	1.1417	-0.7206	0.0000	C	-2.5144	1.3955	0.0000	H	5.8234	-1.4110	0.0000
C	2.4149	-1.4137	0.0000	C	-4.9722	-1.4209	0.0000	H	5.8136	1.4513	0.0000
C	3.6914	-0.6562	0.0000	C	-6.1462	-0.7334	0.0000	H	4.6590	3.8848	0.0000
C	3.6869	0.6817	0.0000	C	-6.1512	0.6911	0.0000	H	-7.1137	1.2129	0.0000
C	2.4051	1.4303	0.0000	C	-4.9819	1.3866	0.0000	H	-7.1051	-1.2619	0.0000
C	1.1367	0.7284	0.0000	C	2.7207	-2.7413	0.0000	H	-4.9584	-2.5167	0.0000
C	-0.0414	-1.4051	0.0000	C	4.7643	-1.6587	0.0000	H	-4.9756	2.4825	0.0000
C	-1.2958	-0.7152	0.0000	C	4.1849	-2.8865	0.0000	H	-2.5019	-2.5098	0.0000
C	-1.3007	0.7063	0.0000	C	2.7016	2.7599	0.0000	H	-2.5192	2.4925	0.0000
C	-0.0511	1.4048	0.0000	C	4.7527	1.6916	0.0000	H	-0.0521	-2.5025	0.0000
C	-2.5047	-1.4128	0.0000	C	4.1648	2.9153	0.0000	H	-0.0693	2.5021	0.0000
C	-3.7212	-0.7232	0.0000	H	2.0335	-3.5856	0.0000	H	2.0085	3.5993	0.0000
C	-3.7262	0.6975	0.0000	H	4.6858	-3.8525	0.0000				

Table 3.167: Table of thermodynamic data as a function of temperature for Dicyclopenta[*a,c*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.369	630.442	630.442	∞
100	103.955	335.441	734.484	-39.904	652.598	691.847	-361.377
200	199.367	435.143	560.028	-24.977	640.843	735.785	-192.163
250	255.407	485.601	540.076	-13.619	635.325	760.159	-158.823
298.15	310.122	535.278	535.278	0.000	630.442	784.658	-137.466
300	312.197	537.203	535.284	0.576	630.263	785.613	-136.785
350	366.635	589.461	539.286	17.561	625.801	811.869	-121.162
400	416.908	641.752	548.829	37.169	621.962	838.711	-109.522
450	462.276	693.525	562.037	59.170	618.664	866.007	-100.521
500	502.702	744.365	577.737	83.314	615.822	893.663	-93.358
600	570.281	842.241	613.741	137.100	611.233	949.687	-82.676
700	623.605	934.312	653.032	196.896	607.911	1006.381	-75.096
800	666.348	1020.473	693.637	261.469	605.709	1063.458	-69.435
900	701.200	1101.037	734.478	329.903	604.486	1120.747	-65.045
1000	730.020	1176.454	774.946	401.509	604.111	1178.136	-61.538
1100	754.116	1247.196	814.696	475.750	604.423	1235.538	-58.670
1200	774.438	1313.708	853.537	552.206	605.309	1292.868	-56.276
1300	791.699	1376.397	891.369	630.536	606.616	1350.117	-54.247
1400	806.452	1435.622	928.148	710.463	608.235	1407.256	-52.504
1500	819.132	1491.704	963.866	791.758	610.098	1464.272	-50.989
1600	830.089	1544.928	998.533	874.232	612.095	1521.150	-49.659
1700	839.602	1595.544	1032.175	957.727	614.164	1577.880	-48.481
1800	847.903	1643.775	1064.824	1042.112	616.243	1634.545	-47.432
1900	855.178	1689.818	1096.516	1127.274	618.305	1691.047	-46.489
2000	861.582	1733.849	1127.290	1213.118	620.303	1747.466	-45.638
2100	867.242	1776.025	1157.185	1299.565	622.172	1803.775	-44.866
2200	872.266	1816.488	1186.240	1386.546	623.912	1860.000	-44.161
2300	876.740	1855.362	1214.492	1474.000	625.517	1916.148	-43.516
2400	880.741	1892.762	1241.979	1561.878	626.928	1972.188	-42.923
2500	884.330	1928.789	1268.736	1650.135	628.155	2028.274	-42.378
2600	887.560	1963.538	1294.795	1738.732	629.166	2084.210	-41.871
2700	890.476	1997.090	1320.188	1827.636	629.966	2140.176	-41.403
2800	893.117	2029.523	1344.945	1916.818	630.533	2196.136	-40.969
2900	895.515	2060.906	1369.095	2006.251	630.840	2252.033	-40.563
3000	897.698	2091.303	1392.665	2095.914	630.928	2307.946	-40.184
3100	899.692	2120.771	1415.679	2185.785	630.727	2363.794	-39.829
3200	901.516	2149.364	1438.162	2275.846	630.274	2419.716	-39.497
3300	903.189	2177.132	1460.137	2366.083	629.555	2475.692	-39.186
3400	904.727	2204.118	1481.624	2456.480	628.544	2531.617	-38.893
3500	906.144	2230.364	1502.643	2547.024	627.245	2587.560	-38.616
3600	907.452	2255.910	1523.214	2637.705	625.679	2643.621	-38.357
3700	908.662	2280.790	1543.354	2728.511	623.817	2699.745	-38.113
3800	909.783	2305.037	1563.081	2819.434	621.637	2755.869	-37.881
3900	910.824	2328.683	1582.410	2910.465	619.175	2812.010	-37.662
4000	911.791	2351.755	1601.356	3001.596	616.417	2868.340	-37.456
4100	912.692	2374.281	1619.934	3092.821	613.330	2924.677	-37.260
4200	913.533	2396.285	1638.158	3184.133	609.941	2981.086	-37.074
4300	914.318	2417.790	1656.040	3275.526	606.236	3037.500	-36.898
4400	915.053	2438.818	1673.592	3366.995	602.224	3094.084	-36.731
4500	915.741	2459.390	1690.826	3458.535	597.917	3150.813	-36.573
4600	916.387	2479.524	1707.754	3550.142	593.270	3207.648	-36.423
4700	916.994	2499.238	1724.385	3641.811	588.295	3264.487	-36.280
4800	917.564	2518.550	1740.730	3733.539	583.034	3321.529	-36.145
4900	918.101	2537.475	1756.797	3825.323	577.422	3378.564	-36.015
5000	918.607	2556.029	1772.597	3917.158	571.541	3435.882	-35.894

3.168. Cyclopent[*i*]indeno[5,6-*a*]anthracene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 222-88-8
Point Group: C_s

Length: 16.60 Å
Width: 9.747 Å
Breadth: 3.888 Å
L/B Ratio: 1.703

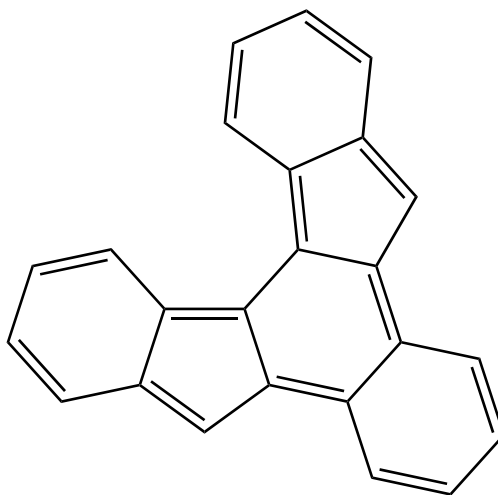
Cartesian coordinates:

C	4.4987	2.5219	0.0000	C	-0.5067	0.6067	0.0000	H	-5.2308	3.1898	0.0000
C	3.6774	1.3082	0.0000	C	-1.8449	0.3768	0.0000	H	4.0939	3.5310	0.0000
C	4.6229	0.1775	0.0000	C	-2.3630	-0.9884	0.0000	H	6.8290	0.1240	0.0000
C	5.8950	0.6810	0.0000	C	-1.3997	-2.0649	0.0000	H	6.6786	2.7924	0.0000
C	5.8069	2.1413	0.0000	C	-2.7858	1.4897	0.0000	H	-4.0934	-2.2681	0.0000
C	4.1040	-1.1538	0.0000	C	-4.1039	1.2288	0.0000	H	-2.3938	2.5132	0.0000
C	2.7548	-1.3504	0.0000	C	-4.6252	-0.1519	0.0000	H	-1.7841	-3.0931	0.0000
C	1.8138	-0.2350	0.0000	C	-3.7031	-1.2440	0.0000	H	-0.1134	1.6369	0.0000
C	2.3461	1.1172	0.0000	C	-5.2808	2.1035	0.0000	H	0.4882	-3.9448	0.0000
C	0.4580	-0.4694	0.0000	C	-6.3902	1.3136	0.0000	H	2.9278	-3.5293	0.0000
C	-0.0621	-1.8283	0.0000	C	-5.9918	-0.0944	0.0000	H	4.8067	-1.9946	0.0000
C	0.8893	-2.9246	0.0000	H	-7.4280	1.6408	0.0000	H	1.6368	1.9584	0.0000
C	2.2132	-2.6976	0.0000	H	-6.6909	-0.9278	0.0000				

Table 3.168: Table of thermodynamic data as a function of temperature for Cyclopent[*i*]indeno[5,6-*a*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.715	690.240	690.240	∞
100	103.116	346.066	747.731	-40.166	712.134	750.321	-391.919
200	200.880	445.886	571.926	-25.208	700.410	793.203	-207.159
250	257.826	496.785	551.785	-13.750	694.992	817.030	-170.705
298.15	313.117	546.941	546.941	0.000	690.240	840.979	-147.333
300	315.209	548.884	546.947	0.581	690.066	841.912	-146.587
350	369.982	601.635	550.988	17.726	685.765	867.571	-129.475
400	420.402	654.384	560.619	37.506	682.097	893.793	-116.715
450	465.785	706.571	573.944	59.682	678.974	920.447	-106.840
500	506.139	757.778	589.776	84.001	676.307	947.441	-98.976
600	573.430	856.256	626.062	138.117	672.048	1002.093	-87.238
700	626.397	948.786	665.629	198.210	669.023	1057.361	-78.900
800	668.792	1035.298	706.492	263.045	667.083	1112.973	-72.668
900	703.329	1116.131	747.567	331.707	666.088	1168.765	-67.832
1000	731.877	1191.757	788.246	403.512	665.912	1224.634	-63.967
1100	755.742	1262.665	828.186	477.927	666.398	1280.496	-60.804
1200	775.868	1329.310	867.197	554.536	667.437	1336.273	-58.165
1300	792.962	1392.106	905.183	633.000	668.878	1391.956	-55.928
1400	807.574	1451.420	942.101	713.045	670.616	1447.519	-54.006
1500	820.134	1507.576	977.945	794.446	672.585	1502.952	-52.336
1600	830.987	1560.861	1012.726	877.015	674.677	1558.240	-50.870
1700	840.413	1611.528	1046.472	960.596	676.831	1613.375	-49.572
1800	848.636	1659.803	1079.215	1045.058	678.987	1668.438	-48.416
1900	855.845	1705.884	1110.994	1130.290	681.119	1723.336	-47.377
2000	862.190	1749.948	1141.848	1216.198	683.181	1778.146	-46.439
2100	867.799	1792.152	1171.818	1302.703	685.108	1832.844	-45.589
2200	872.777	1832.640	1200.941	1389.737	686.901	1887.455	-44.813
2300	877.212	1871.536	1229.257	1477.241	688.556	1941.987	-44.103
2400	881.177	1908.955	1256.803	1565.164	690.012	1996.409	-43.450
2500	884.734	1945.000	1283.615	1653.462	691.281	2050.874	-42.850
2600	887.935	1979.763	1309.725	1742.099	692.331	2105.189	-42.293
2700	890.826	2013.329	1335.167	1831.039	693.167	2159.531	-41.778
2800	893.443	2045.775	1359.969	1920.255	693.768	2213.867	-41.299
2900	895.821	2077.169	1384.162	2009.720	694.107	2268.138	-40.853
3000	897.985	2107.576	1407.772	2099.412	694.224	2322.424	-40.436
3100	899.961	2137.053	1430.824	2189.311	694.051	2376.644	-40.045
3200	901.769	2165.655	1453.343	2279.398	693.625	2430.938	-39.680
3300	903.428	2193.429	1475.351	2369.659	692.930	2485.284	-39.338
3400	904.953	2220.422	1496.869	2460.080	691.942	2539.579	-39.015
3500	906.357	2246.675	1517.919	2550.646	690.665	2593.891	-38.711
3600	907.654	2272.226	1538.519	2641.347	689.119	2648.321	-38.425
3700	908.854	2297.112	1558.686	2732.174	687.278	2702.813	-38.156
3800	909.965	2321.364	1578.439	2823.115	685.116	2757.305	-37.901
3900	910.997	2345.014	1597.793	2914.164	682.672	2811.813	-37.659
4000	911.956	2368.091	1616.763	3005.312	679.930	2866.510	-37.432
4100	912.849	2390.621	1635.364	3096.553	676.860	2921.213	-37.216
4200	913.683	2412.628	1653.609	3187.880	673.486	2975.987	-37.011
4300	914.461	2434.137	1671.512	3279.288	669.796	3030.766	-36.816
4400	915.190	2455.169	1689.084	3370.771	665.798	3085.716	-36.631
4500	915.872	2475.743	1706.338	3462.324	661.504	3140.810	-36.457
4600	916.513	2495.880	1723.284	3553.944	656.870	3196.009	-36.291
4700	917.114	2515.597	1739.932	3645.625	651.907	3251.213	-36.132
4800	917.680	2534.912	1756.294	3737.365	646.658	3306.618	-35.983
4900	918.212	2553.839	1772.378	3829.160	641.057	3362.017	-35.839
5000	918.714	2572.395	1788.193	3921.007	635.187	3417.699	-35.704

3.169. Benz[*a*]indeno[2,1-*c*]naphthalene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 193-27-1
Point Group: C₂

Length: 13.33 Å
Width: 12.40 Å
Breadth: 4.228 Å
L/B Ratio: 1.074

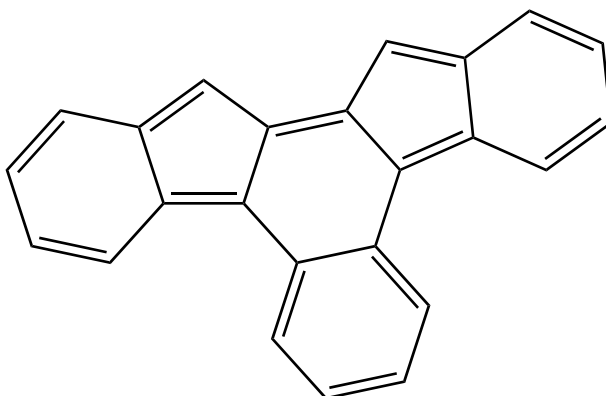
Cartesian coordinates:

C	-2.6671	-1.6915	0.2000	C	3.5183	1.3914	0.0719	H	-3.3045	5.0450	-0.0420
C	-1.2953	-1.7201	0.0398	C	4.7198	0.6948	0.0369	H	-0.8145	5.1254	0.1731
C	-0.6337	-2.9777	-0.0731	C	4.7198	-0.6944	-0.0369	H	-3.2083	0.7500	-0.3490
C	-1.3349	-4.1677	-0.0787	C	3.5185	-1.3911	-0.0719	H	1.5436	3.5468	0.2062
C	-2.7264	-4.1152	0.0489	C	0.8080	2.7466	0.1296	H	3.5231	2.4863	0.1278
C	-3.3763	-2.8985	0.1963	C	-0.6339	2.9776	0.0731	H	5.6681	1.2411	0.0668
C	0.8083	-2.7465	-0.1296	C	-1.3353	4.1676	0.0787	H	5.6682	-1.2408	-0.0668
C	1.0355	-1.4071	-0.0535	C	-2.7267	4.1150	-0.0489	H	3.5228	-2.4860	-0.1278
C	-0.2609	-0.6733	0.0056	C	-3.3765	2.8983	-0.1963	H	-0.8142	-5.1255	-0.1731
C	-0.2609	0.6733	-0.0056	C	-2.6673	1.6913	-0.2000	H	-3.3041	-5.0453	0.0420
C	1.0354	1.4072	0.0535	C	-1.2955	1.7199	-0.0398	H	-4.4649	-2.8767	0.3146
C	2.3023	0.7041	0.0344	H	1.5438	-3.5468	-0.2062	H	-3.2083	-0.7503	0.3490
C	2.3023	-0.7039	-0.0344	H	-4.4651	2.8763	-0.3146				

Table 3.169: Table of thermodynamic data as a function of temperature for Benz[*a*]indeno[2,1-*c*]naphthalene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.932	530.392	530.392	∞
100	103.362	337.474	731.330	-39.386	553.066	592.113	-309.282
200	196.615	436.112	559.232	-24.624	541.146	635.894	-166.075
250	251.731	485.849	539.562	-13.428	535.466	660.238	-137.946
298.15	305.947	534.830	534.830	0.000	530.392	684.741	-119.961
300	308.010	536.729	534.836	0.568	530.205	685.698	-119.388
350	362.306	588.327	538.787	17.339	525.529	711.994	-106.257
400	412.677	640.045	548.213	36.732	521.476	738.907	-96.489
450	458.275	691.332	561.272	58.527	517.971	766.301	-88.948
500	498.990	741.765	576.808	82.478	514.936	794.077	-82.955
600	567.168	839.017	612.479	135.923	510.006	850.394	-74.032
700	621.021	930.649	651.456	195.435	506.400	907.434	-67.712
800	664.198	1016.495	691.780	259.772	503.962	964.894	-63.000
900	699.395	1096.827	732.371	328.010	502.542	1022.593	-59.349
1000	728.491	1172.068	772.620	399.449	502.001	1080.413	-56.434
1100	752.808	1242.675	812.176	473.549	502.172	1138.259	-54.050
1200	773.308	1309.081	850.845	549.883	502.936	1196.047	-52.062
1300	790.715	1371.685	888.525	628.107	504.138	1253.763	-50.376
1400	805.588	1430.842	925.169	707.942	505.664	1311.377	-48.927
1500	818.368	1486.868	960.765	789.155	507.445	1368.874	-47.667
1600	829.408	1540.045	995.322	871.557	509.370	1426.239	-46.561
1700	838.993	1590.622	1028.864	954.988	511.376	1483.459	-45.580
1800	847.355	1638.820	1061.423	1039.315	513.396	1540.617	-44.707
1900	854.682	1684.835	1093.032	1124.425	515.406	1597.617	-43.921
2000	861.131	1728.841	1123.730	1210.222	517.357	1654.535	-43.211
2100	866.831	1770.997	1153.556	1296.626	519.183	1711.345	-42.567
2200	871.889	1811.441	1182.547	1383.567	520.883	1768.074	-41.979
2300	876.394	1850.299	1210.740	1470.986	522.453	1824.728	-41.440
2400	880.422	1887.685	1238.172	1558.830	523.830	1881.275	-40.944
2500	884.034	1923.700	1264.878	1647.056	525.026	1937.869	-40.489
2600	887.286	1958.437	1290.889	1735.625	526.009	1994.315	-40.065
2700	890.221	1991.979	1316.238	1824.503	526.783	2050.792	-39.674
2800	892.879	2024.403	1340.953	1913.660	527.325	2107.263	-39.311
2900	895.293	2055.779	1365.065	2003.070	527.610	2163.672	-38.971
3000	897.491	2086.168	1388.598	2092.711	527.675	2220.099	-38.655
3100	899.497	2115.630	1411.577	2182.562	527.454	2276.460	-38.357
3200	901.332	2144.217	1434.028	2272.605	526.983	2332.897	-38.080
3300	903.016	2171.979	1455.971	2362.824	526.246	2389.387	-37.820
3400	904.564	2198.960	1477.429	2453.204	525.218	2445.828	-37.575
3500	905.990	2225.202	1498.421	2543.732	523.903	2502.287	-37.344
3600	907.306	2250.743	1518.966	2634.398	522.322	2558.865	-37.127
3700	908.524	2275.619	1539.081	2725.190	520.446	2615.505	-36.924
3800	909.652	2299.863	1558.784	2816.100	518.253	2672.147	-36.730
3900	910.699	2323.505	1578.090	2907.118	515.778	2728.805	-36.547
4000	911.673	2346.574	1597.015	2998.237	513.007	2785.654	-36.376
4100	912.580	2369.097	1615.573	3089.450	509.909	2842.509	-36.213
4200	913.425	2391.099	1633.777	3180.751	506.509	2899.436	-36.059
4300	914.216	2412.601	1651.640	3272.134	502.794	2956.368	-35.912
4400	914.955	2433.627	1669.174	3363.592	498.772	3013.472	-35.774
4500	915.647	2454.197	1686.392	3455.123	494.455	3070.720	-35.643
4600	916.297	2474.329	1703.303	3546.721	489.799	3128.075	-35.520
4700	916.907	2494.041	1719.918	3638.381	484.815	3185.433	-35.401
4800	917.481	2513.352	1736.247	3730.101	479.546	3242.994	-35.290
4900	918.022	2532.275	1752.300	3821.876	473.925	3300.549	-35.184
5000	918.531	2550.827	1768.086	3913.704	468.036	3358.388	-35.084

3.170. Benz[*c*]indeno[2,1-*a*]fluorene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 201-72-9
Point Group: C_{2v}

Length: 15.05 Å
Width: 10.46 Å
Breadth: 3.889 Å
L/B Ratio: 1.438

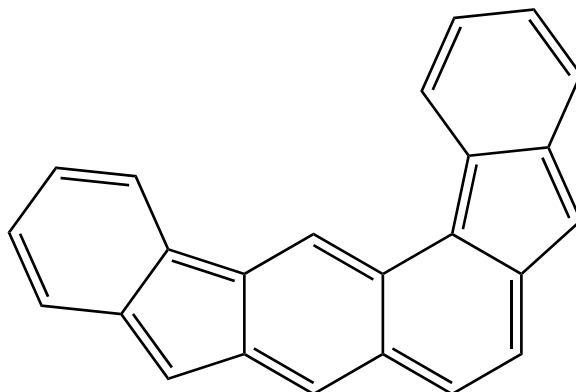
Cartesian coordinates:

C	-4.1994	-2.1880	0.0000	C	0.7374	3.7927	0.0000	H	6.1495	0.5562	0.0000
C	-2.9639	-1.5702	0.0000	C	-0.7011	3.7996	0.0000	H	3.9408	1.6916	0.0000
C	-2.8472	-0.1483	0.0000	C	-1.3927	2.6421	0.0000	H	4.2498	-3.3199	0.0000
C	-3.9873	0.6331	0.0000	C	-1.6210	-2.1509	0.0000	H	1.3852	-3.2332	0.0000
C	-5.2364	0.0020	0.0000	C	1.6004	-2.1662	0.0000	H	2.5172	2.6255	0.0000
C	-5.3425	-1.3818	0.0000	C	2.9488	-1.5984	0.0000	H	1.2603	4.7547	0.0000
C	-1.4129	0.1760	0.0000	C	4.1783	-2.2280	0.0000	H	-1.2148	4.7666	0.0000
C	-0.7198	-1.1279	0.0000	C	5.3290	-1.4328	0.0000	H	-2.4920	2.6494	0.0000
C	0.7090	-1.1347	0.0000	C	5.2362	-0.0481	0.0000	H	-3.9244	1.7292	0.0000
C	1.4145	0.1625	0.0000	C	3.9932	0.5950	0.0000	H	-6.1439	0.6150	0.0000
C	0.7402	1.3479	0.0000	C	2.8457	-0.1755	0.0000	H	-6.3316	-1.8514	0.0000
C	-0.7272	1.3549	0.0000	H	-1.4160	-3.2198	0.0000	H	-4.2814	-3.2791	0.0000
C	1.4179	2.6286	0.0000	H	6.3136	-1.9118	0.0000				

Table 3.170: Table of thermodynamic data as a function of temperature for Benz[*c*]indeno[2,1-*a*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.631	601.189	601.189	∞
100	105.027	344.279	742.793	-39.851	623.398	661.764	-345.663
200	199.115	444.321	568.731	-24.882	611.685	704.792	-184.069
250	254.392	494.638	548.862	-13.556	606.135	728.710	-152.252
298.15	308.577	544.087	544.087	0.000	601.189	752.779	-131.881
300	310.636	546.002	544.093	0.573	601.007	753.718	-131.231
350	364.795	597.995	548.075	17.472	596.460	779.540	-116.338
400	414.987	650.034	557.570	36.986	592.526	805.962	-105.246
450	460.394	701.582	570.714	58.891	589.132	832.849	-96.673
500	500.921	752.229	586.342	82.943	586.199	860.108	-89.853
600	568.755	849.802	622.196	136.563	581.444	915.361	-79.688
700	622.315	941.656	661.343	196.219	577.982	971.310	-72.479
800	665.251	1027.659	701.817	260.673	575.661	1027.662	-67.098
900	700.253	1108.102	742.540	329.006	574.335	1084.238	-62.926
1000	729.194	1183.426	782.903	400.523	573.872	1140.926	-59.595
1100	753.388	1254.094	822.560	474.687	574.107	1197.634	-56.870
1200	773.790	1320.546	861.318	551.074	574.924	1254.278	-54.596
1300	791.119	1383.185	899.076	629.342	576.170	1310.845	-52.669
1400	805.929	1442.369	935.788	709.214	577.733	1367.307	-51.014
1500	818.659	1498.418	971.445	790.459	579.546	1423.651	-49.575
1600	829.659	1551.612	1006.057	872.888	581.498	1479.859	-48.311
1700	839.210	1602.203	1039.649	956.343	583.527	1535.922	-47.192
1800	847.544	1650.413	1072.252	1040.690	585.568	1591.922	-46.195
1900	854.848	1696.437	1103.902	1125.817	587.595	1647.761	-45.299
2000	861.278	1740.452	1134.637	1211.630	589.563	1703.519	-44.490
2100	866.962	1782.614	1164.496	1298.048	591.402	1759.168	-43.756
2200	872.006	1823.064	1193.518	1385.001	593.115	1814.735	-43.086
2300	876.500	1861.927	1221.740	1472.431	594.695	1870.227	-42.473
2400	880.517	1899.317	1249.198	1560.285	596.083	1925.610	-41.909
2500	884.121	1935.336	1275.928	1648.520	597.288	1981.041	-41.391
2600	887.365	1970.076	1301.962	1737.098	598.279	2036.323	-40.909
2700	890.294	2003.621	1327.331	1825.983	599.060	2091.636	-40.464
2800	892.946	2036.048	1352.067	1915.147	599.609	2146.943	-40.051
2900	895.354	2067.425	1376.196	2004.564	599.900	2202.187	-39.665
3000	897.547	2097.817	1399.747	2094.211	599.972	2257.449	-39.305
3100	899.549	2127.280	1422.743	2184.067	599.756	2312.645	-38.967
3200	901.381	2155.869	1445.208	2274.115	599.290	2367.917	-38.651
3300	903.062	2183.632	1467.166	2364.338	598.558	2423.242	-38.356
3400	904.607	2210.615	1488.637	2454.723	597.534	2478.518	-38.077
3500	906.030	2236.858	1509.642	2545.256	596.224	2533.811	-37.814
3600	907.344	2262.400	1530.199	2635.925	594.647	2589.223	-37.568
3700	908.559	2287.277	1550.325	2726.721	592.774	2644.698	-37.336
3800	909.685	2311.522	1570.039	2817.634	590.584	2700.174	-37.116
3900	910.730	2335.165	1589.356	2908.655	588.113	2755.666	-36.907
4000	911.702	2358.235	1608.291	2999.778	585.345	2811.348	-36.712
4100	912.608	2380.759	1626.858	3090.994	582.250	2867.037	-36.526
4200	913.452	2402.761	1645.071	3182.297	578.852	2922.798	-36.350
4300	914.241	2424.264	1662.943	3273.682	575.140	2978.564	-36.182
4400	914.979	2445.290	1680.485	3365.144	571.120	3034.502	-36.023
4500	915.670	2465.860	1697.710	3456.676	566.806	3090.584	-35.874
4600	916.319	2485.993	1714.629	3548.276	562.152	3146.772	-35.732
4700	916.928	2505.706	1731.251	3639.939	557.170	3202.964	-35.596
4800	917.501	2525.017	1747.587	3731.661	551.903	3259.358	-35.468
4900	918.041	2543.941	1763.647	3823.438	546.284	3315.747	-35.346
5000	918.549	2562.493	1779.439	3915.268	540.397	3372.419	-35.231

3.171. Fluoreno[3,4-*b*]fluorene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 198-93-6
Point Group: C_s

Length: 15.01 Å
Width: 10.62 Å
Breadth: 3.886 Å
L/B Ratio: 1.412

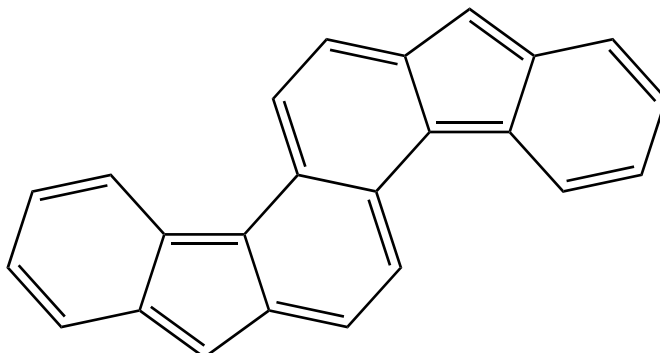
Cartesian coordinates:

C	2.2352	2.1139	0.0000	C	-1.1483	-2.5479	0.0000	H	-6.6530	1.9167	0.0000
C	2.6371	0.7909	0.0000	C	-2.1695	-1.5406	0.0000	H	-6.2257	-0.5420	0.0000
C	4.0256	0.4668	0.0000	C	-1.7609	-0.1218	0.0000	H	-2.4106	2.7294	0.0000
C	4.9888	1.4584	0.0000	C	-0.4698	0.2474	0.0000	H	-4.1374	-2.5369	0.0000
C	4.5665	2.7910	0.0000	C	-3.5305	-1.6333	0.0000	H	-1.4543	-3.6006	0.0000
C	3.2150	3.1117	0.0000	C	-4.0822	-0.2761	0.0000	H	-0.1717	1.3063	0.0000
C	4.1672	-0.9892	0.0000	C	-5.3920	0.1667	0.0000	H	0.8591	-4.2575	0.0000
C	2.9197	-1.5369	0.0000	C	-5.6224	1.5463	0.0000	H	3.2814	-3.6895	0.0000
C	1.8924	-0.4738	0.0000	C	-4.5686	2.4518	0.0000	H	6.0536	1.2062	0.0000
C	0.5680	-0.7726	0.0000	C	-3.2392	2.0142	0.0000	H	5.3137	3.5915	0.0000
C	0.1626	-2.1857	0.0000	C	-3.0034	0.6542	0.0000	H	2.9078	4.1628	0.0000
C	1.1953	-3.2137	0.0000	H	5.1234	-1.5090	0.0000	H	1.1695	2.3793	0.0000
C	2.5076	-2.9152	0.0000	H	-4.7784	3.5266	0.0000				

Table 3.171: Table of thermodynamic data as a function of temperature for Fluoreno[3,4-*b*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-46.028	565.440	565.440	∞
100	102.105	344.362	739.433	-39.507	587.992	626.350	-327.165
200	197.431	442.655	566.569	-24.783	576.035	669.474	-174.845
250	253.435	492.679	546.766	-13.522	570.420	693.484	-144.893
298.15	308.066	542.001	542.001	0.000	565.440	717.651	-125.727
300	310.137	543.913	542.007	0.572	565.256	718.594	-125.116
350	364.532	595.850	545.985	17.453	560.690	744.522	-111.112
400	414.829	647.861	555.471	36.956	556.747	771.052	-100.687
450	460.275	699.394	568.606	58.855	553.346	798.048	-92.633
500	500.816	750.029	584.225	82.902	550.407	825.416	-86.229
600	568.669	847.584	620.064	136.512	545.643	880.891	-76.687
700	622.267	939.427	659.197	196.161	542.174	937.062	-69.923
800	665.252	1025.427	699.661	260.613	539.850	993.637	-64.877
900	700.304	1105.873	740.376	328.948	538.527	1050.436	-60.964
1000	729.287	1181.204	780.733	400.472	538.071	1107.347	-57.841
1100	753.513	1251.883	820.385	474.647	538.318	1164.276	-55.286
1200	773.938	1318.347	859.141	551.048	539.149	1221.141	-53.154
1300	791.282	1380.999	896.897	629.332	540.410	1277.927	-51.347
1400	806.100	1440.196	933.610	709.220	541.990	1334.608	-49.794
1500	818.833	1496.256	969.267	790.483	543.821	1391.168	-48.444
1600	829.833	1549.462	1003.881	872.929	545.790	1447.592	-47.258
1700	839.381	1600.063	1037.474	956.401	547.836	1503.869	-46.207
1800	847.711	1648.282	1070.079	1040.765	549.894	1560.082	-45.271
1900	855.009	1694.315	1101.732	1125.909	551.938	1616.135	-44.430
2000	861.433	1738.338	1132.469	1211.738	553.920	1672.104	-43.670
2100	867.110	1780.508	1162.331	1298.171	555.775	1727.964	-42.980
2200	872.148	1820.964	1191.356	1385.139	557.502	1783.742	-42.351
2300	876.635	1859.834	1219.581	1472.582	559.097	1839.442	-41.774
2400	880.646	1897.229	1247.042	1560.450	560.497	1895.035	-41.244
2500	884.243	1933.253	1273.774	1648.697	561.715	1950.674	-40.756
2600	887.481	1967.998	1299.811	1737.286	562.718	2006.165	-40.304
2700	890.404	2001.548	1325.184	1826.183	563.511	2061.685	-39.885
2800	893.051	2033.978	1349.922	1915.358	564.071	2117.199	-39.496
2900	895.454	2065.359	1374.054	2004.785	564.372	2172.650	-39.133
3000	897.642	2095.754	1397.607	2094.442	564.453	2228.118	-38.794
3100	899.640	2125.221	1420.605	2184.307	564.247	2283.521	-38.476
3200	901.468	2153.812	1443.073	2274.364	563.790	2338.998	-38.179
3300	903.144	2181.578	1465.034	2364.596	563.065	2394.529	-37.901
3400	904.685	2208.563	1486.507	2454.988	562.050	2450.010	-37.639
3500	906.105	2234.808	1507.514	2545.529	560.747	2505.508	-37.392
3600	907.415	2260.352	1528.073	2636.206	559.177	2561.125	-37.160
3700	908.628	2285.231	1548.202	2727.009	557.312	2616.805	-36.942
3800	909.751	2309.478	1567.918	2817.928	555.129	2672.485	-36.735
3900	910.793	2333.123	1587.237	2908.956	552.664	2728.182	-36.539
4000	911.762	2356.195	1606.173	3000.084	549.902	2784.068	-36.355
4100	912.665	2378.720	1624.742	3091.306	546.813	2839.961	-36.181
4200	913.507	2400.723	1642.957	3182.615	543.421	2895.926	-36.015
4300	914.294	2422.227	1660.831	3274.006	539.714	2951.896	-35.858
4400	915.030	2443.255	1678.375	3365.473	535.699	3008.037	-35.709
4500	915.719	2463.826	1695.602	3457.010	531.390	3064.322	-35.569
4600	916.366	2483.960	1712.522	3548.615	526.741	3120.713	-35.436
4700	916.974	2503.674	1729.146	3640.282	521.764	3177.109	-35.309
4800	917.545	2522.985	1745.484	3732.008	516.501	3233.707	-35.189
4900	918.083	2541.910	1761.545	3823.790	510.887	3290.298	-35.074
5000	918.590	2560.463	1777.338	3915.624	505.004	3347.173	-34.967

3.172. Fluoreno[4,3-*c*]fluorene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 131238-65-8
Point Group: C_{2h}

Length: 16.20 Å
Width: 9.244 Å
Breadth: 3.885 Å
L/B Ratio: 1.752

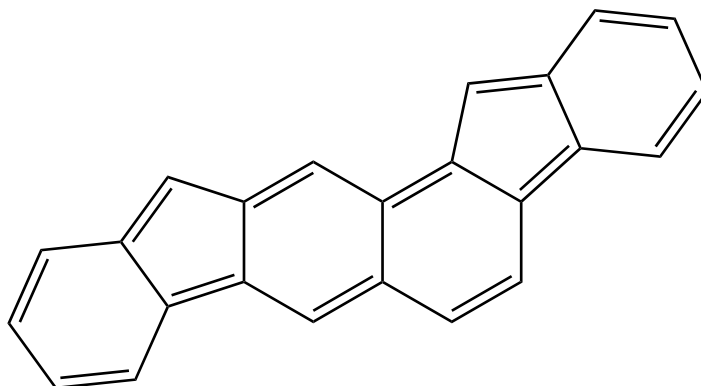
Cartesian coordinates:

C	-3.2050	-0.2610	0.0000	C	3.2050	0.2610	0.0000	H	-6.0748	1.6410	0.0000
C	-1.8166	0.2198	0.0000	C	4.0529	-0.8856	0.0000	H	-3.1246	-2.4234	0.0000
C	-1.9126	1.6940	0.0000	C	3.2177	-2.0859	0.0000	H	-3.6089	3.1017	0.0000
C	-3.2177	2.0859	0.0000	C	3.7597	1.5275	0.0000	H	-0.7964	3.5699	0.0000
C	-4.0529	0.8855	0.0000	C	5.1531	1.6504	0.0000	H	1.4172	2.4435	0.0000
C	-0.6126	-0.4092	0.0000	C	5.9737	0.5301	0.0000	H	0.7964	-3.5699	0.0000
C	0.6127	0.4092	0.0000	C	5.4292	-0.7575	0.0000	H	-1.4172	-2.4435	0.0000
C	0.4865	1.8580	0.0000	C	-3.7598	-1.5276	0.0000	H	3.6080	-3.1020	0.0000
C	-0.7079	2.4785	0.0000	C	-5.1531	-1.6504	0.0000	H	3.1246	2.4233	0.0000
C	1.8166	-0.2198	0.0000	C	-5.9736	-0.5301	0.0000	H	5.6011	2.6497	0.0000
C	1.9126	-1.6939	0.0000	C	-5.4292	0.7575	0.0000	H	7.0616	0.6540	0.0000
C	0.7079	-2.4785	0.0000	H	-5.6012	-2.6497	0.0000	H	6.0749	-1.6409	0.0000
C	-0.4865	-1.8580	0.0000	H	-7.0616	-0.6539	0.0000				

Table 3.172: Table of thermodynamic data as a function of temperature for Fluoreno[4,3-*c*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-46.452	576.467	576.467	∞
100	103.416	348.330	745.123	-39.679	598.848	636.809	-332.628
200	198.287	447.328	571.606	-24.856	586.990	679.495	-177.462
250	254.178	497.532	551.749	-13.554	581.415	703.266	-146.936
298.15	308.678	546.973	546.973	0.000	576.467	727.196	-127.399
300	310.745	548.889	546.979	0.573	576.285	728.130	-126.776
350	365.015	600.910	550.964	17.481	571.747	753.807	-112.497
400	415.210	652.979	560.464	37.006	567.824	780.082	-101.866
450	460.574	704.551	573.615	58.921	564.441	806.822	-93.652
500	501.047	755.214	589.251	82.982	561.515	833.931	-87.118
600	568.788	852.801	625.119	136.609	556.768	888.886	-77.383
700	622.292	944.656	664.277	196.265	553.306	944.535	-70.481
800	665.200	1030.653	704.759	260.716	550.981	1000.586	-65.330
900	700.191	1111.090	745.487	329.042	549.650	1056.864	-61.338
1000	729.129	1186.407	785.854	400.553	549.180	1113.253	-58.149
1100	753.325	1257.069	825.514	474.710	549.409	1169.663	-55.542
1200	773.731	1323.516	864.273	551.092	550.220	1226.010	-53.366
1300	791.065	1386.150	902.032	629.354	551.460	1282.280	-51.522
1400	805.880	1445.331	938.745	709.221	553.018	1338.446	-49.937
1500	818.614	1501.376	974.402	790.461	554.827	1394.494	-48.560
1600	829.618	1554.568	1009.014	872.886	556.774	1450.407	-47.350
1700	839.173	1605.157	1042.606	956.337	558.799	1506.174	-46.278
1800	847.511	1653.364	1075.208	1040.680	560.837	1561.878	-45.324
1900	854.818	1699.386	1106.858	1125.804	562.861	1617.423	-44.465
2000	861.251	1743.400	1137.592	1211.615	564.825	1672.885	-43.690
2100	866.937	1785.561	1167.451	1298.030	566.662	1728.240	-42.987
2200	871.983	1826.009	1196.473	1384.981	568.372	1783.513	-42.345
2300	876.478	1864.872	1224.694	1472.408	569.950	1838.709	-41.758
2400	880.497	1902.261	1252.152	1560.260	571.336	1893.799	-41.217
2500	884.103	1938.279	1278.881	1648.494	572.539	1948.935	-40.720
2600	887.348	1973.018	1304.915	1737.069	573.528	2003.923	-40.258
2700	890.278	2006.563	1330.284	1825.953	574.308	2058.941	-39.832
2800	892.931	2038.989	1355.019	1915.115	574.856	2113.954	-39.435
2900	895.340	2070.366	1379.148	2004.531	575.145	2168.905	-39.065
3000	897.534	2100.757	1402.698	2094.176	575.216	2223.872	-38.720
3100	899.537	2130.220	1425.694	2184.031	574.999	2278.775	-38.396
3200	901.370	2158.808	1448.159	2274.078	574.531	2333.753	-38.094
3300	903.051	2186.571	1470.117	2364.300	573.798	2388.784	-37.811
3400	904.597	2213.553	1491.587	2454.684	572.773	2443.765	-37.543
3500	906.020	2239.796	1512.592	2545.215	571.462	2498.765	-37.291
3600	907.335	2265.338	1533.148	2635.884	569.883	2553.883	-37.055
3700	908.550	2290.215	1553.275	2726.679	568.010	2609.064	-36.833
3800	909.677	2314.459	1572.988	2817.591	565.819	2664.246	-36.622
3900	910.723	2338.102	1592.305	2908.612	563.347	2719.445	-36.422
4000	911.695	2361.172	1611.239	2999.733	560.579	2774.833	-36.235
4100	912.600	2383.696	1629.806	3090.948	557.483	2830.229	-36.057
4200	913.445	2405.697	1648.019	3182.251	554.085	2885.696	-35.888
4300	914.234	2427.201	1665.890	3273.636	550.371	2941.169	-35.727
4400	914.973	2448.227	1683.432	3365.096	546.351	2996.812	-35.576
4500	915.664	2468.797	1700.657	3456.629	542.036	3052.600	-35.433
4600	916.313	2488.929	1717.575	3548.228	537.381	3108.495	-35.297
4700	916.923	2508.642	1734.198	3639.890	532.399	3164.393	-35.168
4800	917.496	2527.953	1750.534	3731.611	527.132	3220.494	-35.045
4900	918.036	2546.876	1766.593	3823.388	521.513	3276.589	-34.928
5000	918.545	2565.428	1782.385	3915.217	515.625	3332.968	-34.819

3.173. Fluoreno[2,3-*a*]fluorene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 223-66-5
Point Group: C_s

Length: 17.37 Å
Width: 8.647 Å
Breadth: 3.886 Å
L/B Ratio: 2.009

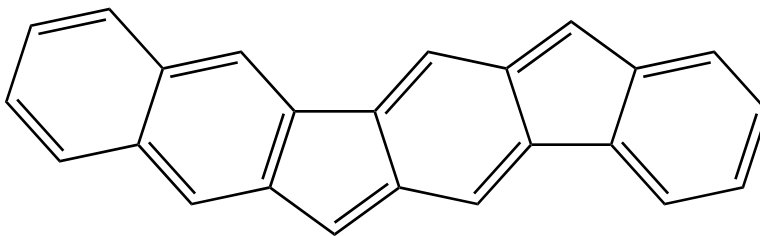
Cartesian coordinates:

C	-5.0981	-1.7812	0.0000	C	1.6040	1.4773	0.0000	H	7.0163	1.6316	0.0000
C	-3.9399	-1.0264	0.0000	C	2.4384	0.4250	0.0000	H	4.6277	2.3632	0.0000
C	-4.0026	0.3962	0.0000	C	1.9438	-0.9669	0.0000	H	5.8221	-2.5182	0.0000
C	-5.2171	1.0531	0.0000	C	0.5275	-1.1936	0.0000	H	2.9633	-2.9229	0.0000
C	-6.3833	0.2800	0.0000	C	2.9963	-1.8350	0.0000	H	1.9761	2.5087	0.0000
C	-6.3242	-1.1083	0.0000	C	4.2348	-1.0533	0.0000	H	0.1600	-2.2263	0.0000
C	-2.5321	-1.4312	0.0000	C	5.5577	-1.4564	0.0000	H	-0.3018	3.3358	0.0000
C	-1.7599	-0.3048	0.0000	C	6.5485	-0.4697	0.0000	H	-2.7644	3.0247	0.0000
C	-2.6252	0.8908	0.0000	C	6.2195	0.8804	0.0000	H	-5.2656	2.1465	0.0000
C	-2.1194	2.1397	0.0000	C	4.8845	1.2992	0.0000	H	-7.3573	0.7802	0.0000
C	-0.6903	2.3102	0.0000	C	3.9000	0.3313	0.0000	H	-7.2530	-1.6884	0.0000
C	0.1646	1.2497	0.0000	H	-2.2018	-2.4687	0.0000	H	-5.0572	-2.8746	0.0000
C	-0.3250	-0.1333	0.0000	H	7.6019	-0.7690	0.0000				

Table 3.173: Table of thermodynamic data as a function of temperature for Fluoreno[2,3-*a*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-46.023	567.404	567.404	∞
100	102.593	343.233	738.383	-39.515	589.949	628.420	-328.246
200	197.411	441.733	565.552	-24.764	578.019	671.642	-175.411
250	253.220	491.729	545.766	-13.509	572.397	695.699	-145.355
298.15	307.781	541.006	541.006	0.000	567.404	719.912	-126.123
300	309.852	542.916	541.012	0.571	567.221	720.857	-125.510
350	364.259	594.809	544.986	17.438	562.641	746.837	-111.457
400	414.609	646.787	554.464	36.929	558.684	773.419	-100.996
450	460.122	698.297	567.591	58.818	555.274	800.470	-92.914
500	500.731	748.920	583.201	82.859	552.330	827.893	-86.488
600	568.702	846.470	619.025	136.467	547.563	883.479	-76.912
700	622.387	938.326	658.148	196.124	544.102	939.761	-70.124
800	665.434	1024.345	698.606	260.591	541.794	996.445	-65.060
900	700.527	1104.816	739.320	328.947	540.491	1053.352	-61.134
1000	729.535	1180.172	779.678	400.494	540.059	1110.367	-57.998
1100	753.773	1250.875	819.334	474.695	540.331	1167.398	-55.434
1200	774.202	1317.362	858.094	551.122	541.188	1224.362	-53.294
1300	791.542	1380.035	895.856	629.433	542.475	1281.246	-51.480
1400	806.354	1439.250	932.574	709.347	544.081	1338.022	-49.921
1500	819.078	1495.328	968.239	790.634	545.936	1394.676	-48.566
1600	830.066	1548.549	1002.859	873.104	547.930	1451.192	-47.376
1700	839.603	1599.165	1036.459	956.599	549.998	1507.560	-46.321
1800	847.921	1647.396	1069.071	1040.984	552.078	1563.862	-45.381
1900	855.208	1693.440	1100.730	1126.149	554.142	1620.002	-44.536
2000	861.621	1737.473	1131.474	1211.997	556.144	1676.059	-43.773
2100	867.287	1779.651	1161.343	1298.448	558.018	1732.005	-43.080
2200	872.314	1820.116	1190.374	1385.433	559.762	1787.868	-42.448
2300	876.792	1858.993	1218.604	1472.893	561.372	1843.653	-41.870
2400	880.793	1896.395	1246.071	1560.776	562.788	1899.330	-41.337
2500	884.383	1932.424	1272.809	1649.038	564.020	1955.051	-40.848
2600	887.613	1967.175	1298.851	1737.640	565.037	2010.625	-40.393
2700	890.529	2000.729	1324.229	1826.550	565.842	2066.227	-39.973
2800	893.168	2033.164	1348.972	1915.737	566.414	2121.823	-39.582
2900	895.565	2064.549	1373.109	2005.175	566.727	2177.355	-39.218
3000	897.748	2094.947	1396.666	2094.843	566.819	2232.904	-38.878
3100	899.740	2124.417	1419.669	2184.718	566.623	2288.387	-38.558
3200	901.562	2153.012	1442.142	2274.785	566.175	2343.945	-38.260
3300	903.234	2180.781	1464.106	2365.026	565.460	2399.556	-37.981
3400	904.771	2207.768	1485.583	2455.427	564.454	2455.116	-37.717
3500	906.186	2234.016	1506.594	2545.976	563.160	2510.694	-37.469
3600	907.493	2259.562	1527.156	2636.661	561.597	2566.390	-37.237
3700	908.702	2284.443	1547.289	2727.471	559.740	2622.148	-37.017
3800	909.821	2308.692	1567.008	2818.398	557.564	2677.907	-36.810
3900	910.861	2332.339	1586.330	2909.433	555.105	2733.682	-36.613
4000	911.827	2355.412	1605.270	3000.568	552.350	2789.647	-36.428
4100	912.727	2377.938	1623.842	3091.796	549.268	2845.618	-36.253
4200	913.566	2399.943	1642.059	3183.111	545.882	2901.661	-36.087
4300	914.351	2421.449	1659.936	3274.508	542.180	2957.709	-35.928
4400	915.084	2442.478	1677.483	3365.980	538.171	3013.928	-35.779
4500	915.771	2463.050	1694.712	3457.523	533.867	3070.291	-35.638
4600	916.416	2483.185	1711.635	3549.133	529.223	3126.760	-35.505
4700	917.022	2502.900	1728.261	3640.805	524.251	3183.232	-35.377
4800	917.591	2522.213	1744.601	3732.536	518.993	3239.908	-35.257
4900	918.127	2541.138	1760.665	3824.322	513.383	3296.576	-35.141
5000	918.633	2559.692	1776.460	3916.160	507.505	3353.528	-35.033

3.174. Benz[*b*]indeno[2,1-*h*]fluorene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 102634-38-8
Point Group: C_s

Length: 17.87 Å
Width: 8.387 Å
Breadth: 3.883 Å
L/B Ratio: 2.131

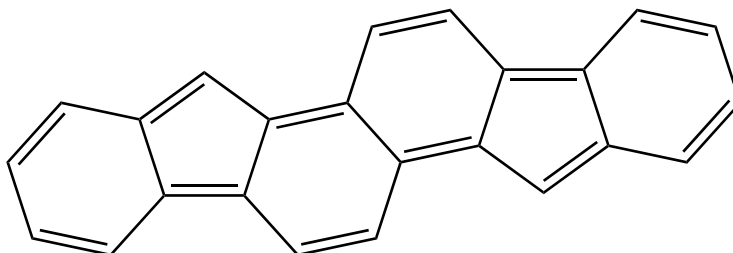
Cartesian coordinates:

C	-5.7076	-1.3900	0.0000	C	0.7774	2.0412	0.0000	H	5.9713	2.0286	0.0000
C	-4.3767	-1.0148	0.0000	C	2.0073	1.2451	0.0000	H	4.6948	-2.7942	0.0000
C	-4.0117	0.3614	0.0000	C	3.3152	1.6281	0.0000	H	3.6056	2.6841	0.0000
C	-4.9759	1.3502	0.0000	C	4.3223	0.6153	0.0000	H	2.3121	-2.1937	0.0000
C	-6.3193	0.9601	0.0000	C	3.9611	-0.7505	0.0000	H	0.7618	3.1299	0.0000
C	-6.6773	-0.3827	0.0000	C	2.5840	-1.1324	0.0000	H	-2.0513	2.5157	0.0000
C	-3.1548	-1.8227	0.0000	C	1.6389	-0.1527	0.0000	H	-0.3214	-2.3009	0.0000
C	-2.0829	-0.9810	0.0000	C	5.6965	0.9676	0.0000	H	-3.1467	-2.9112	0.0000
C	-0.6677	-1.2624	0.0000	C	6.6627	-0.0046	0.0000	H	-4.6963	2.4084	0.0000
C	0.1759	-0.2124	0.0000	C	6.3015	-1.3691	0.0000	H	-7.0999	1.7281	0.0000
C	-0.2893	1.1948	0.0000	C	4.9809	-1.7362	0.0000	H	-7.7368	-0.6594	0.0000
C	-1.7054	1.4770	0.0000	H	7.0893	-2.1296	0.0000	H	-5.9943	-2.4460	0.0000
C	-2.5486	0.4273	0.0000	H	7.7235	0.2667	0.0000				

Table 3.174: Table of thermodynamic data as a function of temperature for Benz[*b*]indeno[2,1-*h*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.662	518.400	518.400	∞
100	100.950	340.684	733.498	-39.281	541.178	579.904	-302.904
200	196.273	438.201	561.546	-24.669	529.108	623.439	-162.822
250	252.270	487.965	541.830	-13.466	523.435	647.678	-135.322
298.15	306.939	537.084	537.084	0.000	518.400	672.077	-117.743
300	309.012	538.989	537.090	0.570	518.214	673.029	-117.182
350	363.470	590.757	541.054	17.396	513.594	699.208	-104.349
400	413.839	642.631	550.511	36.848	509.599	725.996	-94.803
450	459.363	694.051	563.610	58.699	506.150	753.256	-87.434
500	499.984	744.595	579.190	82.702	503.168	780.894	-81.578
600	568.003	842.013	614.950	136.238	498.328	836.919	-72.859
700	621.757	933.765	654.011	195.828	494.801	893.653	-66.684
800	664.880	1019.706	694.411	260.236	492.434	950.797	-62.079
900	700.046	1100.116	735.071	328.540	491.079	1008.170	-58.511
1000	729.119	1175.424	775.382	400.043	490.602	1065.658	-55.663
1100	753.414	1246.090	814.995	474.205	490.835	1123.166	-53.334
1200	773.890	1312.548	853.716	550.598	491.659	1180.610	-51.390
1300	791.271	1375.198	891.444	628.880	492.917	1237.976	-49.741
1400	806.117	1434.395	928.132	708.768	494.498	1295.237	-48.325
1500	818.869	1490.457	963.768	790.033	496.331	1352.377	-47.093
1600	829.881	1543.665	998.363	872.484	498.305	1409.381	-46.011
1700	839.439	1594.270	1031.940	955.961	500.356	1466.238	-45.051
1800	847.773	1642.492	1064.531	1040.331	502.420	1523.030	-44.196
1900	855.075	1688.529	1096.170	1125.482	504.470	1579.661	-43.427
2000	861.501	1732.555	1126.897	1211.317	506.460	1636.209	-42.733
2100	867.178	1774.728	1156.749	1297.757	508.321	1692.647	-42.101
2200	872.215	1815.188	1185.765	1384.731	510.055	1749.002	-41.526
2300	876.701	1854.060	1213.982	1472.181	511.656	1805.281	-40.998
2400	880.710	1891.459	1241.436	1560.056	513.063	1861.451	-40.513
2500	884.306	1927.485	1268.161	1648.310	514.287	1917.667	-40.067
2600	887.542	1962.233	1294.192	1736.905	515.296	1973.734	-39.652
2700	890.463	1995.784	1319.559	1825.808	516.095	2029.830	-39.269
2800	893.107	2028.217	1344.293	1914.988	516.661	2085.921	-38.913
2900	895.509	2059.600	1368.420	2004.421	516.967	2141.948	-38.580
3000	897.695	2089.996	1391.969	2094.083	517.054	2197.992	-38.270
3100	899.690	2119.465	1414.964	2183.953	516.853	2253.970	-37.978
3200	901.516	2148.058	1437.428	2274.015	516.401	2310.023	-37.706
3300	903.190	2175.825	1459.385	2364.252	515.681	2366.130	-37.452
3400	904.730	2202.811	1480.856	2454.649	514.670	2422.185	-37.212
3500	906.148	2229.058	1501.860	2545.193	513.372	2478.259	-36.985
3600	907.456	2254.603	1522.416	2635.875	511.806	2534.451	-36.773
3700	908.667	2279.483	1542.542	2726.681	509.945	2590.705	-36.573
3800	909.788	2303.731	1562.256	2817.605	507.766	2646.960	-36.384
3900	910.829	2327.377	1581.573	2908.636	505.304	2703.232	-36.205
4000	911.797	2350.449	1600.507	2999.768	502.546	2759.692	-36.037
4100	912.699	2372.975	1619.074	3090.994	499.460	2816.160	-35.878
4200	913.539	2394.979	1637.287	3182.306	496.072	2872.699	-35.727
4300	914.325	2416.485	1655.159	3273.700	492.367	2929.243	-35.583
4400	915.060	2437.513	1672.702	3365.169	488.356	2985.959	-35.447
4500	915.748	2458.085	1689.927	3456.710	484.050	3042.818	-35.319
4600	916.394	2478.219	1706.846	3548.318	479.403	3099.783	-35.198
4700	917.000	2497.934	1723.468	3639.988	474.429	3156.753	-35.083
4800	917.571	2517.246	1739.805	3731.716	469.169	3213.925	-34.974
4900	918.108	2536.171	1755.865	3823.501	463.557	3271.090	-34.870
5000	918.614	2554.724	1771.657	3915.337	457.676	3328.539	-34.772

3.175. Fluoreno[2,1-*a*]fluorene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 221-15-8
Point Group: C_{2h}

Length: 17.20 Å
Width: 7.970 Å
Breadth: 3.884 Å
L/B Ratio: 2.158

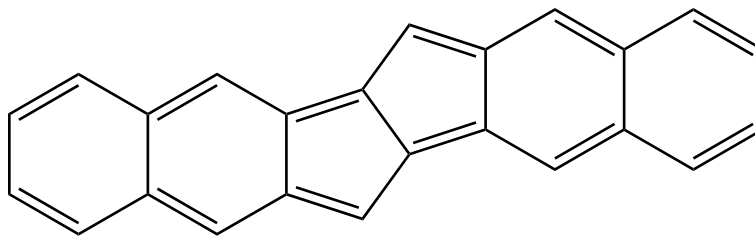
Cartesian coordinates:

C	-4.9636	-1.4110	0.0000	C	0.2840	1.8345	0.0000	H	4.8148	2.4953	0.0000
C	-3.8869	-0.5464	0.0000	C	1.7210	1.9230	0.0000	H	5.5129	-2.4815	0.0000
C	-4.0815	0.8641	0.0000	C	2.4431	0.7853	0.0000	H	2.6319	-2.5956	0.0000
C	-5.3566	1.3985	0.0000	C	1.8070	-0.5463	0.0000	H	2.1965	2.9094	0.0000
C	-6.4416	0.5161	0.0000	C	2.7695	-1.5154	0.0000	H	-0.2849	2.7720	0.0000
C	-6.2497	-0.8601	0.0000	C	4.0815	-0.8641	0.0000	H	-2.1966	-2.9094	0.0000
C	-2.7696	1.5154	0.0000	C	5.3565	-1.3986	0.0000	H	0.2849	-2.7719	0.0000
C	-1.8070	0.5463	0.0000	C	6.4417	-0.5162	0.0000	H	-2.6317	2.5956	0.0000
C	-0.3643	0.6364	0.0000	C	6.2498	0.8601	0.0000	H	-5.5130	2.4815	0.0000
C	0.3643	-0.6364	0.0000	C	4.9636	1.4110	0.0000	H	-7.4596	0.9197	0.0000
C	-0.2841	-1.8345	0.0000	C	3.8870	0.5464	0.0000	H	-7.1179	-1.5275	0.0000
C	-1.7211	-1.9229	0.0000	H	7.4597	-0.9198	0.0000	H	-4.8147	-2.4953	0.0000
C	-2.4431	-0.7853	0.0000	H	7.1180	1.5274	0.0000				

Table 3.175: Table of thermodynamic data as a function of temperature for Fluoreno[2,1-*a*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-46.247	584.961	584.961	∞
100	103.725	339.999	736.301	-39.630	607.391	646.184	-337.525
200	197.961	439.142	563.091	-24.790	595.549	689.691	-180.125
250	253.456	489.225	543.289	-13.516	589.947	713.875	-149.153
298.15	307.846	538.527	538.527	0.000	584.961	738.208	-129.328
300	309.912	540.437	538.533	0.571	584.777	739.158	-128.696
350	364.255	592.333	542.507	17.439	580.198	765.260	-114.207
400	414.602	644.310	551.986	36.930	576.242	791.967	-103.418
450	460.138	695.821	565.113	58.819	572.832	819.141	-95.082
500	500.776	746.447	580.723	82.862	569.889	846.689	-88.451
600	568.791	844.010	616.549	136.476	565.128	902.521	-78.570
700	622.495	935.880	655.676	196.143	561.677	959.049	-71.564
800	665.544	1021.915	696.138	260.621	559.380	1015.976	-66.335
900	700.629	1102.398	736.856	328.988	558.088	1073.125	-62.281
1000	729.626	1177.764	777.219	400.545	557.666	1130.381	-59.044
1100	753.852	1248.475	816.880	474.754	557.946	1187.653	-56.396
1200	774.270	1314.969	855.645	551.189	558.811	1244.857	-54.186
1300	791.601	1377.646	893.411	629.505	560.104	1301.980	-52.313
1400	806.405	1436.866	930.134	709.425	561.716	1358.994	-50.704
1500	819.121	1492.947	965.802	790.717	563.576	1415.886	-49.305
1600	830.104	1546.171	1000.426	873.191	565.573	1472.640	-48.076
1700	839.636	1596.788	1034.030	956.689	567.645	1529.246	-46.987
1800	847.949	1645.021	1066.645	1041.078	569.728	1585.786	-46.017
1900	855.233	1691.067	1098.306	1126.245	571.795	1642.164	-45.145
2000	861.643	1735.101	1129.053	1212.095	573.799	1698.457	-44.358
2100	867.307	1777.281	1158.924	1298.549	575.675	1754.640	-43.643
2200	872.332	1817.746	1187.957	1385.536	577.420	1810.740	-42.992
2300	876.807	1856.623	1216.190	1472.997	579.033	1866.763	-42.395
2400	880.808	1894.026	1243.659	1560.881	580.450	1922.676	-41.845
2500	884.396	1930.056	1270.399	1649.145	581.683	1978.635	-41.340
2600	887.624	1964.807	1296.442	1737.748	582.701	2034.445	-40.872
2700	890.539	1998.362	1321.822	1826.659	583.508	2090.284	-40.438
2800	893.178	2030.797	1346.566	1915.847	584.081	2146.116	-40.035
2900	895.574	2062.182	1370.704	2005.287	584.394	2201.886	-39.659
3000	897.756	2092.581	1394.263	2094.955	584.488	2257.671	-39.309
3100	899.747	2122.051	1417.267	2184.831	584.292	2313.391	-38.980
3200	901.570	2150.646	1439.741	2274.899	583.845	2369.185	-38.672
3300	903.241	2178.415	1461.706	2365.140	583.131	2425.032	-38.384
3400	904.777	2205.403	1483.184	2455.542	582.125	2480.829	-38.113
3500	906.192	2231.651	1504.196	2546.092	580.832	2536.643	-37.857
3600	907.498	2257.197	1524.759	2636.777	579.270	2592.576	-37.617
3700	908.707	2282.079	1544.893	2727.588	577.413	2648.571	-37.390
3800	909.826	2306.327	1564.613	2818.515	575.237	2704.566	-37.176
3900	910.865	2329.974	1583.935	2909.551	572.779	2760.578	-36.973
4000	911.831	2353.047	1602.876	3000.686	570.025	2816.779	-36.783
4100	912.731	2375.574	1621.449	3091.915	566.942	2872.987	-36.602
4200	913.570	2397.579	1639.667	3183.230	563.557	2929.266	-36.430
4300	914.354	2419.085	1657.544	3274.627	559.856	2985.550	-36.266
4400	915.088	2440.114	1675.091	3366.099	555.847	3042.006	-36.112
4500	915.775	2460.686	1692.321	3457.643	551.544	3098.605	-35.967
4600	916.419	2480.821	1709.245	3549.253	546.900	3155.310	-35.829
4700	917.025	2500.537	1725.872	3640.925	541.928	3212.019	-35.697
4800	917.594	2519.849	1742.212	3732.656	536.670	3268.931	-35.572
4900	918.130	2538.775	1758.276	3824.443	531.061	3325.836	-35.453
5000	918.635	2557.329	1774.072	3916.281	525.182	3383.024	-35.341

3.176. Pentaleno[1,2-*b*:4,5-*b'*]dinaphthalene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 155121-10-1
Point Group: C_{2h}

Length: 17.88 Å
Width: 7.848 Å
Breadth: 3.883 Å
L/B Ratio: 2.279

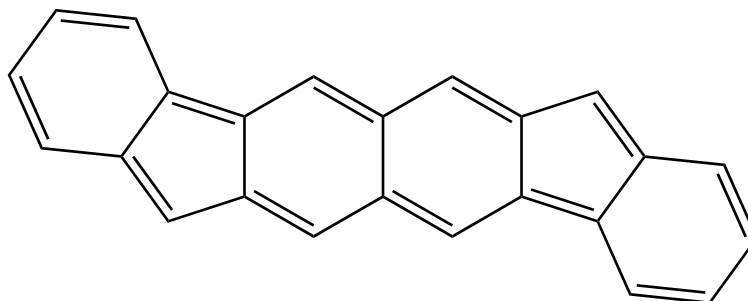
Cartesian coordinates:

C	-5.6151	-1.2728	0.0000	C	0.5923	1.6573	0.0000	H	5.7343	2.3624	0.0000
C	-4.3073	-0.7260	0.0000	C	1.9247	1.0213	0.0000	H	5.1665	-2.5934	0.0000
C	-4.1467	0.6769	0.0000	C	3.1631	1.5847	0.0000	H	3.3013	2.6712	0.0000
C	-5.2969	1.5053	0.0000	C	4.3073	0.7260	0.0000	H	2.7252	-2.3435	0.0000
C	-6.5517	0.9515	0.0000	C	4.1468	-0.6768	0.0000	H	0.4398	2.7348	0.0000
C	-6.7122	-0.4497	0.0000	C	2.8375	-1.2542	0.0000	H	-0.4394	-2.7349	0.0000
C	-2.8375	1.2542	0.0000	C	1.7623	-0.4220	0.0000	H	-2.7251	2.3434	0.0000
C	-1.7623	0.4219	0.0000	C	5.6151	1.2729	0.0000	H	-3.3014	-2.6712	0.0000
C	-1.9247	-1.0214	0.0000	C	6.7121	0.4498	0.0000	H	-5.1665	2.5935	0.0000
C	-3.1631	-1.5847	0.0000	C	6.5517	-0.9515	0.0000	H	-7.4404	1.5911	0.0000
C	-0.5923	-1.6574	0.0000	C	5.2969	-1.5052	0.0000	H	-7.7225	-0.8718	0.0000
C	0.3305	-0.6724	0.0000	H	7.4404	-1.5910	0.0000	H	-5.7343	-2.3623	0.0000
C	-0.3304	0.6723	0.0000	H	7.7224	0.8719	0.0000				

Table 3.176: Table of thermodynamic data as a function of temperature for Pentaleno[1,2-*b*:4,5-*b'*]dinaphthalene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.846	502.909	502.909	∞
100	101.718	339.782	733.035	-39.325	525.644	564.460	-294.837
200	196.384	437.634	560.977	-24.669	513.619	608.062	-158.806
250	252.244	487.404	541.263	-13.465	507.947	632.330	-132.115
298.15	306.908	536.517	536.517	0.000	502.909	656.756	-115.058
300	308.983	538.422	536.523	0.570	502.724	657.709	-114.515
350	363.487	590.189	540.487	17.396	498.103	683.916	-102.067
400	413.907	642.069	549.944	36.850	494.110	710.732	-92.810
450	459.470	693.499	563.044	58.705	490.666	738.021	-85.665
500	500.116	744.055	578.626	82.715	487.690	765.686	-79.989
600	568.154	841.500	614.392	136.264	482.865	821.764	-71.539
700	621.908	933.275	653.461	195.870	479.352	878.547	-65.557
800	665.023	1019.236	693.870	260.292	477.000	935.739	-61.096
900	700.179	1099.662	734.539	328.610	475.659	993.159	-57.640
1000	729.242	1174.984	774.858	400.126	475.195	1050.691	-54.881
1100	753.527	1245.661	814.479	474.300	475.440	1108.243	-52.625
1200	773.995	1312.129	853.209	550.704	476.275	1165.729	-50.742
1300	791.367	1374.786	890.943	628.996	477.543	1223.137	-49.145
1400	806.205	1433.990	927.637	708.893	479.133	1280.438	-47.773
1500	818.951	1490.058	963.280	790.167	480.974	1337.619	-46.579
1600	829.956	1543.271	997.880	872.625	482.956	1394.662	-45.530
1700	839.508	1593.881	1031.463	956.110	485.014	1451.558	-44.600
1800	847.838	1642.107	1064.059	1040.486	487.085	1508.389	-43.771
1900	855.135	1688.147	1095.703	1125.643	489.141	1565.059	-43.026
2000	861.556	1732.176	1126.434	1211.484	491.137	1621.645	-42.352
2100	867.230	1774.352	1156.290	1297.929	493.004	1678.121	-41.740
2200	872.263	1814.814	1185.310	1384.909	494.742	1734.514	-41.182
2300	876.745	1853.688	1213.530	1472.364	496.348	1790.829	-40.670
2400	880.752	1891.088	1240.987	1560.242	497.760	1847.037	-40.199
2500	884.345	1927.116	1267.716	1648.500	498.988	1903.289	-39.766
2600	887.578	1961.865	1293.750	1737.099	500.001	1959.393	-39.364
2700	890.497	1995.418	1319.120	1826.005	500.803	2015.526	-38.992
2800	893.140	2027.852	1343.856	1915.189	501.372	2071.654	-38.646
2900	895.539	2059.236	1367.986	2004.625	501.682	2127.717	-38.324
3000	897.723	2089.634	1391.537	2094.290	501.771	2183.798	-38.023
3100	899.717	2119.103	1414.534	2184.164	501.573	2239.812	-37.740
3200	901.541	2147.697	1437.001	2274.228	501.123	2295.901	-37.476
3300	903.215	2175.465	1458.960	2364.467	500.406	2352.043	-37.229
3400	904.753	2202.452	1480.432	2454.866	499.398	2408.135	-36.996
3500	906.169	2228.699	1501.438	2545.413	498.102	2464.245	-36.776
3600	907.477	2254.245	1521.996	2636.096	496.538	2520.472	-36.570
3700	908.686	2279.126	1542.124	2726.905	494.679	2576.763	-36.377
3800	909.807	2303.374	1561.839	2817.831	492.501	2633.053	-36.193
3900	910.847	2327.020	1581.157	2908.864	490.042	2689.360	-36.019
4000	911.814	2350.093	1600.094	2999.998	487.285	2745.857	-35.856
4100	912.715	2372.619	1618.662	3091.225	484.201	2802.360	-35.702
4200	913.555	2394.624	1636.876	3182.539	480.814	2858.935	-35.555
4300	914.340	2416.129	1654.749	3273.934	477.111	2915.515	-35.416
4400	915.074	2437.158	1672.293	3365.405	473.101	2972.265	-35.285
4500	915.762	2457.730	1689.520	3456.947	468.797	3029.160	-35.161
4600	916.407	2477.865	1706.440	3548.556	464.151	3086.161	-35.044
4700	917.013	2497.580	1723.063	3640.227	459.179	3143.166	-34.932
4800	917.583	2516.892	1739.401	3731.957	453.920	3200.373	-34.826
4900	918.119	2535.818	1755.462	3823.743	448.309	3257.574	-34.725
5000	918.625	2554.371	1771.255	3915.580	442.430	3315.058	-34.631

3.177. Fluoreno[3,2-*b*]fluorene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 102634-40-2
Point Group: C_{2h}

Length: 17.98 Å
Width: 7.928 Å
Breadth: 3.884 Å
L/B Ratio: 2.268

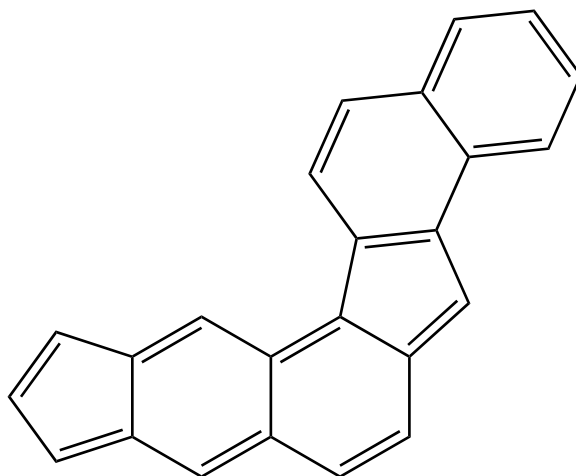
Cartesian coordinates:

C	4.7732	1.5573	0.0000	C	-1.5081	-1.1867	0.0000	H	-4.3429	-2.5636	0.0000
C	3.9627	0.4387	0.0000	C	-2.5067	-0.2886	0.0000	H	-6.3323	2.0512	0.0000
C	4.5232	-0.8707	0.0000	C	-2.2503	1.1659	0.0000	H	-3.5810	2.9254	0.0000
C	5.8954	-1.0480	0.0000	C	-0.8915	1.6244	0.0000	H	-1.7022	-2.2657	0.0000
C	6.7078	0.0891	0.0000	C	-3.4329	1.8472	0.0000	H	-0.7039	2.7045	0.0000
C	6.1585	1.3663	0.0000	C	-4.5231	0.8707	0.0000	H	0.7040	-2.7045	0.0000
C	3.4330	-1.8472	0.0000	C	-5.8954	1.0481	0.0000	H	1.7022	2.2657	0.0000
C	2.2504	-1.1659	0.0000	C	-6.7078	-0.0890	0.0000	H	3.5810	-2.9255	0.0000
C	0.8915	-1.6245	0.0000	C	-6.1585	-1.3662	0.0000	H	6.3324	-2.0512	0.0000
C	-0.1271	-0.7230	0.0000	C	-4.7733	-1.5572	0.0000	H	7.7964	-0.0302	0.0000
C	0.1271	0.7230	0.0000	C	-3.9627	-0.4387	0.0000	H	6.8197	2.2392	0.0000
C	1.5081	1.1866	0.0000	H	-7.7964	0.0304	0.0000	H	4.3427	2.5635	0.0000
C	2.5067	0.2885	0.0000	H	-6.8198	-2.2391	0.0000				

Table 3.177: Table of thermodynamic data as a function of temperature for Fluoreno[3,2-*b*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-45.799	547.580	547.580	∞
100	101.547	337.566	730.850	-39.328	570.312	609.349	-318.285
200	196.478	435.344	558.748	-24.681	558.278	653.179	-170.589
250	252.382	485.143	539.024	-13.470	552.612	677.560	-141.566
298.15	306.988	534.277	534.277	0.000	547.580	702.095	-123.002
300	309.060	536.182	534.283	0.570	547.395	703.052	-122.410
350	363.488	587.954	538.247	17.398	542.776	729.371	-108.850
400	413.856	639.831	547.705	36.850	538.782	756.299	-98.760
450	459.393	691.254	560.804	58.702	535.335	783.700	-90.968
500	500.034	741.801	576.385	82.708	532.354	811.477	-84.773
600	568.088	839.232	612.148	136.250	527.522	867.781	-75.546
700	621.864	930.999	651.213	195.850	524.004	924.792	-69.007
800	664.997	1016.955	691.618	260.269	521.648	982.212	-64.131
900	700.164	1097.378	732.284	328.585	520.305	1039.860	-60.351
1000	729.234	1172.699	772.600	400.099	519.840	1097.620	-57.333
1100	753.523	1243.376	812.219	474.273	520.084	1155.400	-54.864
1200	773.993	1309.843	850.946	550.677	520.918	1213.115	-52.804
1300	791.367	1372.500	888.679	628.968	522.187	1270.752	-51.058
1400	806.205	1431.704	925.371	708.866	523.776	1328.282	-49.558
1500	818.951	1487.772	961.012	790.140	525.618	1385.691	-48.253
1600	829.957	1540.986	995.612	872.598	527.600	1442.963	-47.107
1700	839.508	1591.595	1029.194	956.083	529.658	1500.088	-46.091
1800	847.838	1639.821	1061.788	1040.459	531.729	1557.147	-45.186
1900	855.135	1685.861	1093.432	1125.616	533.785	1614.045	-44.372
2000	861.556	1729.891	1124.162	1211.457	535.781	1670.859	-43.637
2100	867.230	1772.066	1154.018	1297.902	537.648	1727.564	-42.970
2200	872.263	1812.528	1183.036	1384.882	539.386	1784.185	-42.361
2300	876.745	1851.403	1211.256	1472.336	540.992	1840.730	-41.803
2400	880.752	1888.803	1238.713	1560.215	542.403	1897.166	-41.290
2500	884.345	1924.831	1265.442	1648.473	543.631	1953.647	-40.818
2600	887.578	1959.580	1291.475	1737.072	544.644	2009.979	-40.380
2700	890.497	1993.133	1316.845	1825.978	545.447	2066.341	-39.975
2800	893.139	2025.567	1341.580	1915.162	546.015	2122.697	-39.599
2900	895.539	2056.951	1365.710	2004.598	546.325	2178.989	-39.247
3000	897.723	2087.348	1389.261	2094.263	546.415	2235.298	-38.919
3100	899.717	2116.817	1412.257	2184.136	546.217	2291.540	-38.611
3200	901.541	2145.411	1434.724	2274.200	545.767	2347.858	-38.324
3300	903.214	2173.179	1456.682	2364.439	545.050	2404.229	-38.055
3400	904.752	2200.166	1478.155	2454.839	544.041	2460.550	-37.801
3500	906.169	2226.413	1499.160	2545.386	542.745	2516.888	-37.562
3600	907.477	2251.959	1519.718	2636.069	541.181	2573.344	-37.337
3700	908.686	2276.840	1539.846	2726.878	539.322	2629.863	-37.126
3800	909.807	2301.088	1559.561	2817.803	537.145	2686.382	-36.926
3900	910.847	2324.734	1578.879	2908.836	534.685	2742.918	-36.737
4000	911.814	2347.807	1597.815	2999.970	531.928	2799.643	-36.559
4100	912.715	2370.334	1616.383	3091.197	528.844	2856.375	-36.390
4200	913.555	2392.338	1634.597	3182.511	525.457	2913.178	-36.230
4300	914.340	2413.844	1652.470	3273.906	521.755	2969.986	-36.077
4400	915.074	2434.873	1670.014	3365.377	517.745	3026.965	-35.934
4500	915.761	2455.445	1687.240	3456.919	513.440	3084.089	-35.798
4600	916.407	2475.579	1704.160	3548.528	508.794	3141.318	-35.670
4700	917.013	2495.294	1720.784	3640.199	503.822	3198.552	-35.547
4800	917.583	2514.606	1737.121	3731.929	498.563	3255.988	-35.432
4900	918.119	2533.532	1753.182	3823.715	492.952	3313.417	-35.321
5000	918.625	2552.086	1768.975	3915.552	487.073	3371.130	-35.217

3.178. Benz[*a*]indeno[5,6-*g*]fluorene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 192-89-2
Point Group: C_s

Length: 15.89 Å
Width: 9.835 Å
Breadth: 3.888 Å
L/B Ratio: 1.616

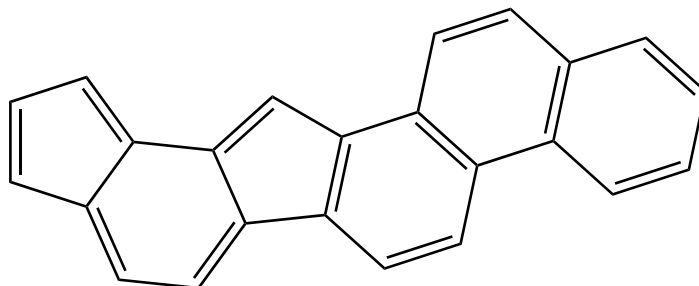
Cartesian coordinates:

C	-4.8424	-1.8383	0.0000	C	1.5925	0.3408	0.0000	H	6.6046	-0.0408	0.0000
C	-3.5294	-1.2897	0.0000	C	2.5431	1.4617	0.0000	H	3.8556	-3.4376	0.0000
C	-3.3749	0.1175	0.0000	C	2.0279	2.8241	0.0000	H	4.6004	2.0854	0.0000
C	-4.5298	0.9463	0.0000	C	0.7092	3.0936	0.0000	H	1.4123	-1.8599	0.0000
C	-5.7785	0.3890	0.0000	C	3.8880	1.2520	0.0000	H	2.7650	3.6359	0.0000
C	-5.9363	-1.0178	0.0000	C	4.3995	-0.0853	0.0000	H	0.3229	4.1178	0.0000
C	-2.0598	0.6320	0.0000	C	3.4479	-1.2114	0.0000	H	-2.5416	-3.2206	0.0000
C	-0.9451	-0.2243	0.0000	C	2.1193	-1.0180	0.0000	H	-0.2407	-2.2807	0.0000
C	-1.1160	-1.6175	0.0000	C	4.2664	-2.4307	0.0000	H	-4.3989	2.0344	0.0000
C	-2.3892	-2.1350	0.0000	C	5.5744	-2.0564	0.0000	H	-6.6710	1.0233	0.0000
C	-1.5957	2.0183	0.0000	C	5.6673	-0.5930	0.0000	H	-6.9473	-1.4383	0.0000
C	-0.2322	2.0076	0.0000	H	-2.2515	2.8875	0.0000	H	-4.9591	-2.9280	0.0000
C	0.2620	0.6133	0.0000	H	6.4449	-2.7091	0.0000				

Table 3.178: Table of thermodynamic data as a function of temperature for Benz[*a*]indeno[5,6-*g*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.671	618.538	618.538	∞
100	104.099	349.224	749.181	-39.996	640.602	678.474	-354.391
200	199.904	449.071	574.294	-25.045	628.871	721.028	-188.309
250	256.118	499.671	554.288	-13.654	623.386	744.702	-155.594
298.15	310.881	549.478	549.478	0.000	618.538	768.520	-134.639
300	312.956	551.407	549.484	0.577	618.360	769.449	-133.970
350	367.388	603.782	553.496	17.600	613.936	794.992	-118.644
400	417.638	656.173	563.059	37.246	610.135	821.115	-107.224
450	462.976	708.030	576.293	59.282	606.872	847.687	-98.395
500	503.371	758.943	592.022	83.461	604.065	874.617	-91.369
600	570.881	856.934	628.085	137.309	599.538	929.177	-80.890
700	624.131	949.092	667.432	197.162	596.273	984.397	-73.455
800	666.805	1035.319	708.089	261.784	594.120	1039.993	-67.903
900	701.593	1115.933	748.976	330.261	592.939	1095.794	-63.597
1000	730.359	1191.389	789.486	401.903	592.601	1151.692	-60.157
1100	754.409	1262.160	829.273	476.176	592.945	1207.598	-57.343
1200	774.692	1328.697	868.147	552.659	593.858	1263.431	-54.995
1300	791.920	1391.404	906.009	631.013	595.189	1319.180	-53.004
1400	806.645	1450.644	942.816	710.960	596.828	1374.817	-51.294
1500	819.303	1506.739	978.557	792.273	598.709	1430.331	-49.808
1600	830.239	1559.974	1013.247	874.763	600.722	1485.705	-48.502
1700	839.737	1610.598	1046.908	958.273	602.806	1540.930	-47.346
1800	848.023	1658.836	1079.575	1042.670	604.897	1596.089	-46.316
1900	855.286	1704.885	1111.283	1127.844	606.971	1651.085	-45.391
2000	861.680	1748.922	1142.072	1213.699	608.980	1705.996	-44.555
2100	867.331	1791.103	1171.981	1300.155	610.858	1760.798	-43.797
2200	872.347	1831.569	1201.049	1387.144	612.606	1815.515	-43.105
2300	876.815	1870.447	1229.314	1474.606	614.219	1870.155	-42.472
2400	880.809	1907.850	1256.812	1562.491	615.637	1924.687	-41.889
2500	884.393	1943.880	1283.578	1650.754	616.870	1979.263	-41.354
2600	887.618	1978.630	1309.647	1739.357	617.887	2033.691	-40.857
2700	890.530	2012.185	1335.049	1828.267	618.693	2088.147	-40.397
2800	893.167	2044.620	1359.815	1917.454	619.265	2142.598	-39.970
2900	895.562	2076.005	1383.973	2006.893	619.578	2196.984	-39.571
3000	897.742	2106.403	1407.550	2096.559	619.669	2251.388	-39.199
3100	899.733	2135.873	1430.571	2186.435	619.473	2305.725	-38.850
3200	901.554	2164.467	1453.061	2276.500	619.024	2360.138	-38.524
3300	903.225	2192.235	1475.041	2366.740	618.308	2414.603	-38.219
3400	904.761	2219.222	1496.534	2457.141	617.301	2469.018	-37.931
3500	906.176	2245.470	1517.559	2547.689	616.006	2523.450	-37.660
3600	907.482	2271.016	1538.135	2638.372	614.442	2578.000	-37.405
3700	908.691	2295.897	1558.280	2729.182	612.584	2632.614	-37.165
3800	909.810	2320.145	1578.012	2820.108	610.407	2687.227	-36.938
3900	910.849	2343.792	1597.345	2911.141	607.947	2741.857	-36.722
4000	911.816	2366.865	1616.296	3002.275	605.191	2796.676	-36.520
4100	912.716	2389.391	1634.878	3093.502	602.107	2851.503	-36.328
4200	913.555	2411.395	1653.106	3184.816	598.720	2906.400	-36.146
4300	914.340	2432.901	1670.991	3276.211	595.017	2961.303	-35.972
4400	915.073	2453.930	1688.547	3367.682	591.007	3016.376	-35.808
4500	915.761	2474.502	1705.785	3459.224	586.702	3071.594	-35.653
4600	916.406	2494.636	1722.716	3550.833	582.057	3126.918	-35.507
4700	917.011	2514.351	1739.351	3642.504	577.084	3182.245	-35.366
4800	917.581	2533.664	1755.698	3734.234	571.825	3237.776	-35.233
4900	918.117	2552.589	1771.769	3826.019	566.214	3293.299	-35.106
5000	918.623	2571.143	1787.571	3917.857	560.335	3349.106	-34.987

3.179. as-Indaceno[2,3-*a*]phenanthrene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 24976-60-1
Point Group: C_s

Length: 16.85 Å
Width: 8.610 Å
Breadth: 3.883 Å
L/B Ratio: 1.957

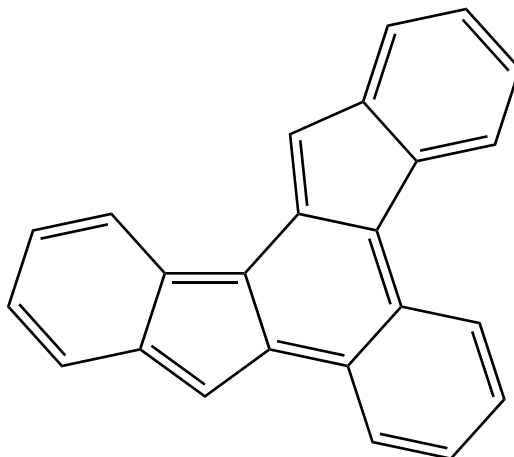
Cartesian coordinates:

C	-5.3616	-1.3238	0.0000	C	0.1762	-0.2653	0.0000	H	4.1783	-2.8960	0.0000
C	-3.9761	-1.0587	0.0000	C	1.3394	-1.1623	0.0000	H	5.1551	2.5250	0.0000
C	-3.5216	0.2718	0.0000	C	2.4669	-0.3984	0.0000	H	2.7160	3.0834	0.0000
C	-4.4692	1.3170	0.0000	C	3.8612	-0.7153	0.0000	H	1.2746	-2.2494	0.0000
C	-5.8182	1.0422	0.0000	C	4.8179	0.4151	0.0000	H	0.1151	3.1693	0.0000
C	-6.2682	-0.2874	0.0000	C	4.4294	1.7051	0.0000	H	-2.3424	2.6867	0.0000
C	-2.0976	0.5415	0.0000	C	3.0146	2.0296	0.0000	H	-3.4140	-3.1658	0.0000
C	-1.1959	-0.5492	0.0000	C	2.1018	1.0386	0.0000	H	-0.9717	-2.7166	0.0000
C	-1.6978	-1.8952	0.0000	C	4.5674	-1.8804	0.0000	H	-4.1048	2.3557	0.0000
C	-3.0283	-2.1398	0.0000	C	6.1542	-0.1977	0.0000	H	-6.5473	1.8590	0.0000
C	-1.6116	1.8631	0.0000	C	5.9993	-1.5475	0.0000	H	-7.3436	-0.4932	0.0000
C	-0.2543	2.1387	0.0000	H	6.7846	-2.3004	0.0000	H	-5.7070	-2.3640	0.0000
C	0.6348	1.0696	0.0000	H	7.0804	0.3721	0.0000				

Table 3.179: Table of thermodynamic data as a function of temperature for as-Indaceno[2,3-*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.401	596.934	596.934	∞
100	103.898	344.375	742.622	-39.825	619.169	657.525	-343.449
200	198.976	443.888	568.519	-24.926	607.385	700.578	-182.968
250	254.883	494.244	548.608	-13.591	601.845	724.518	-151.377
298.15	309.501	543.819	543.819	0.000	596.934	748.603	-131.149
300	311.573	545.740	543.825	0.574	596.753	749.543	-130.504
350	365.977	597.899	547.820	17.527	592.259	775.374	-115.716
400	416.267	650.103	557.345	37.103	588.388	801.796	-104.702
450	461.682	701.803	570.531	59.073	585.058	828.676	-96.188
500	502.169	752.584	586.206	83.189	582.189	855.920	-89.416
600	569.870	850.373	622.161	136.927	577.552	911.127	-79.319
700	623.296	942.388	661.406	196.688	574.194	967.010	-72.158
800	666.119	1028.514	701.972	261.234	571.966	1023.282	-66.812
900	701.030	1109.055	742.778	329.649	570.722	1079.768	-62.667
1000	729.895	1184.456	783.217	401.239	570.333	1136.357	-59.356
1100	754.025	1255.188	822.942	475.470	570.635	1192.958	-56.648
1200	774.371	1321.693	861.761	551.918	571.513	1249.490	-54.388
1300	791.651	1384.377	899.575	630.242	572.814	1305.940	-52.472
1400	806.417	1443.599	936.338	710.165	574.428	1362.281	-50.826
1500	819.107	1499.680	972.042	791.457	576.288	1418.500	-49.396
1600	830.071	1552.902	1006.696	873.929	578.283	1474.581	-48.139
1700	839.591	1603.517	1040.327	957.423	580.352	1530.514	-47.026
1800	847.896	1651.747	1072.966	1041.806	582.429	1586.381	-46.035
1900	855.174	1697.790	1104.649	1126.968	584.491	1642.086	-45.143
2000	861.580	1741.821	1135.415	1212.812	586.489	1697.707	-44.339
2100	867.242	1783.997	1165.302	1299.259	588.358	1753.219	-43.608
2200	872.267	1824.460	1194.351	1386.239	590.097	1808.647	-42.942
2300	876.743	1863.334	1222.597	1473.694	591.703	1863.999	-42.332
2400	880.744	1900.734	1250.079	1561.572	593.114	1919.241	-41.770
2500	884.333	1936.762	1276.830	1649.829	594.341	1974.529	-41.255
2600	887.564	1971.510	1302.884	1738.427	595.353	2029.669	-40.776
2700	890.480	2005.063	1328.273	1827.332	596.153	2084.837	-40.333
2800	893.121	2037.496	1353.026	1916.514	596.721	2140.000	-39.921
2900	895.520	2068.879	1377.173	2005.948	597.029	2195.100	-39.537
3000	897.703	2099.276	1400.739	2095.611	597.116	2250.216	-39.179
3100	899.696	2128.744	1423.750	2185.482	596.916	2305.266	-38.843
3200	901.521	2157.338	1446.230	2275.544	596.464	2360.391	-38.529
3300	903.194	2185.105	1468.202	2365.781	595.745	2415.569	-38.234
3400	904.732	2212.091	1489.686	2456.179	594.734	2470.697	-37.957
3500	906.149	2238.338	1510.703	2546.724	593.436	2525.843	-37.695
3600	907.457	2263.883	1531.271	2637.405	591.870	2581.106	-37.450
3700	908.666	2288.764	1551.409	2728.212	590.009	2636.433	-37.219
3800	909.787	2313.011	1571.134	2819.135	587.830	2691.760	-37.000
3900	910.828	2336.657	1590.460	2910.166	585.368	2747.103	-36.793
4000	911.795	2359.729	1609.405	3001.298	582.610	2802.636	-36.598
4100	912.696	2382.255	1627.981	3092.523	579.524	2858.176	-36.413
4200	913.537	2404.259	1646.203	3183.835	576.135	2913.787	-36.237
4300	914.322	2425.765	1664.083	3275.229	572.430	2969.403	-36.070
4400	915.057	2446.793	1681.634	3366.698	568.419	3025.190	-35.913
4500	915.745	2467.365	1698.867	3458.238	564.112	3081.122	-35.764
4600	916.391	2487.499	1715.793	3549.846	559.465	3137.159	-35.623
4700	916.997	2507.213	1732.423	3641.515	554.491	3193.201	-35.488
4800	917.567	2526.525	1748.766	3733.244	549.231	3249.445	-35.360
4900	918.104	2545.451	1764.833	3825.028	543.618	3305.682	-35.238
5000	918.611	2564.004	1780.631	3916.864	537.737	3362.203	-35.124

3.180. Benz[*a*]indeno[1,2-*c*]fluorene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 199-21-3
Point Group: C_s

Length: 14.31 Å
Width: 11.78 Å
Breadth: 3.886 Å
L/B Ratio: 1.215

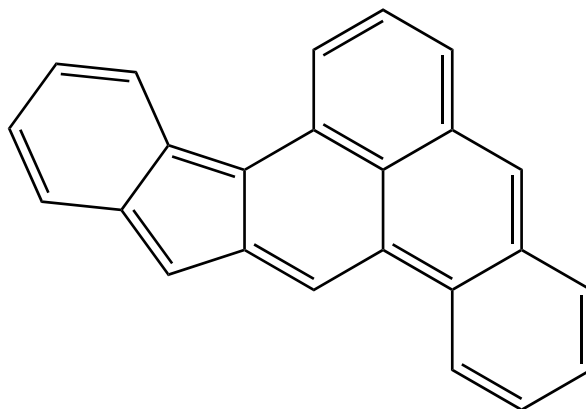
Cartesian coordinates:

C	2.9852	3.1119	0.0000	C	0.6860	-4.3547	0.0000	H	-5.4911	-0.6700	0.0000
C	1.9979	2.0687	0.0000	C	1.9791	-3.8453	0.0000	H	-2.0636	3.0122	0.0000
C	2.4306	0.6563	0.0000	C	2.1894	-2.4721	0.0000	H	-3.1854	-2.4105	0.0000
C	3.8384	0.3793	0.0000	C	-2.6801	-1.4452	0.0000	H	-1.4187	-3.8919	0.0000
C	4.7240	1.4025	0.0000	C	-3.3936	-0.1598	0.0000	H	0.5213	-5.4370	0.0000
C	4.2959	2.7800	0.0000	C	-4.7425	0.1281	0.0000	H	2.8360	-4.5270	0.0000
C	1.3114	-0.1455	0.0000	C	-5.1299	1.4759	0.0000	H	3.2175	-2.0832	0.0000
C	1.1125	-1.5804	0.0000	C	-4.1899	2.4959	0.0000	H	-0.0139	3.0107	0.0000
C	-0.2046	-2.1051	0.0000	C	-2.8166	2.2131	0.0000	H	4.1706	-0.6677	0.0000
C	-1.3395	-1.2013	0.0000	C	-2.4309	0.8897	0.0000	H	5.8015	1.2066	0.0000
C	-1.1090	0.2617	0.0000	C	0.6329	2.1329	0.0000	H	5.0708	3.5537	0.0000
C	0.1377	0.7581	0.0000	H	-4.5205	3.5399	0.0000	H	2.6468	4.1527	0.0000
C	-0.3997	-3.4876	0.0000	H	-6.1969	1.7232	0.0000				

Table 3.180: Table of thermodynamic data as a function of temperature for Benz[*a*]indeno[1,2-*c*]fluorene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.784	601.494	601.494	∞
100	105.512	350.824	750.759	-39.994	623.561	661.272	-345.406
200	199.841	451.239	576.084	-24.969	611.903	703.626	-183.764
250	255.293	501.739	556.146	-13.602	606.394	727.194	-151.936
298.15	309.563	551.355	551.355	0.000	601.494	750.917	-131.555
300	311.624	553.276	551.361	0.575	601.314	751.843	-130.905
350	365.789	605.423	555.355	17.524	596.816	777.297	-116.003
400	415.938	657.592	564.877	37.086	592.931	803.344	-104.904
450	461.277	709.249	578.055	59.037	589.583	829.851	-96.325
500	501.729	759.985	593.721	83.132	586.692	856.724	-89.499
600	569.421	857.692	629.649	136.825	582.011	911.194	-79.325
700	622.869	949.640	668.865	196.542	578.609	966.349	-72.108
800	665.722	1035.711	709.402	261.047	576.340	1021.899	-66.722
900	700.663	1116.206	750.180	329.424	575.058	1077.667	-62.545
1000	729.556	1191.570	790.591	400.979	574.633	1133.543	-59.209
1100	753.711	1262.271	830.291	475.177	574.903	1189.435	-56.480
1200	774.082	1328.750	869.087	551.595	575.750	1245.259	-54.204
1300	791.383	1391.411	906.879	629.891	577.024	1301.005	-52.274
1400	806.170	1450.614	943.623	709.788	578.612	1356.644	-50.616
1500	818.879	1506.679	979.308	791.056	580.449	1412.162	-49.175
1600	829.860	1559.887	1013.945	873.506	582.422	1467.544	-47.909
1700	839.396	1610.490	1047.560	956.980	584.470	1522.779	-46.788
1800	847.715	1658.709	1080.184	1041.345	586.528	1577.949	-45.790
1900	855.006	1704.742	1111.853	1126.489	588.572	1632.959	-44.892
2000	861.425	1748.765	1142.606	1212.317	590.555	1687.885	-44.082
2100	867.098	1790.934	1172.482	1298.749	592.409	1742.703	-43.346
2200	872.132	1831.390	1201.519	1385.716	594.134	1797.437	-42.676
2300	876.617	1870.259	1229.755	1473.157	595.727	1852.096	-42.062
2400	880.627	1907.653	1257.227	1561.023	597.126	1906.647	-41.496
2500	884.224	1943.676	1283.969	1649.269	598.341	1961.243	-40.977
2600	887.461	1978.420	1310.014	1737.856	599.342	2015.691	-40.495
2700	890.384	2011.969	1335.395	1826.751	600.133	2070.169	-40.049
2800	893.030	2044.399	1360.141	1915.923	600.691	2124.641	-39.635
2900	895.434	2075.779	1384.280	2005.349	600.990	2179.050	-39.248
3000	897.622	2106.173	1407.839	2095.003	601.069	2233.477	-38.887
3100	899.620	2135.639	1430.844	2184.867	600.861	2287.837	-38.549
3200	901.448	2164.230	1453.317	2274.921	600.402	2342.273	-38.233
3300	903.125	2191.995	1475.283	2365.151	599.676	2396.762	-37.937
3400	904.667	2218.980	1496.761	2455.542	598.658	2451.201	-37.657
3500	906.087	2245.224	1517.773	2546.081	597.354	2505.658	-37.394
3600	907.398	2270.768	1538.336	2636.756	595.782	2560.233	-37.147
3700	908.611	2295.647	1558.469	2727.557	593.915	2614.871	-36.915
3800	909.734	2319.893	1578.189	2818.475	591.730	2669.510	-36.694
3900	910.777	2343.537	1597.511	2909.501	589.263	2724.165	-36.485
4000	911.747	2366.609	1616.452	3000.628	586.500	2779.010	-36.289
4100	912.650	2389.133	1635.024	3091.848	583.410	2833.861	-36.103
4200	913.493	2411.136	1653.242	3183.156	580.016	2888.785	-35.927
4300	914.280	2432.640	1671.118	3274.545	576.307	2943.713	-35.758
4400	915.016	2453.668	1688.665	3366.010	572.291	2998.813	-35.600
4500	915.706	2474.239	1705.895	3457.547	567.981	3054.057	-35.450
4600	916.353	2494.372	1722.818	3549.150	563.330	3109.407	-35.308
4700	916.961	2514.086	1739.444	3640.816	558.352	3164.761	-35.172
4800	917.533	2533.397	1755.784	3732.541	553.088	3220.318	-35.043
4900	918.071	2552.322	1771.848	3824.321	547.473	3275.868	-34.920
5000	918.579	2570.874	1787.643	3916.154	541.589	3331.702	-34.805

3.181. Fluoreno[4,3,2-*de*]anthracene



Other names: Anthra[9,1-*bc*]fluorene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 195-88-0

Point Group: C_s

Length: 15.59 Å

Width: 10.28 Å

Breadth: 3.884 Å

L/B Ratio: 1.516

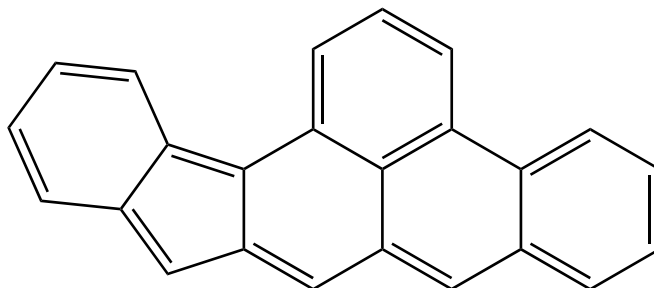
Cartesian coordinates:

C	1.6936	-1.8992	0.0000	C	3.1594	2.0911	0.0000	H	-3.7156	-1.9639	0.0000
C	3.0640	-1.6397	0.0000	C	1.2102	-3.2472	0.0000	H	-4.9472	2.9386	0.0000
C	3.5425	-0.3246	0.0000	C	-0.1273	-3.5007	0.0000	H	-2.0880	3.3507	0.0000
C	2.6305	0.7622	0.0000	C	-1.0635	-2.4356	0.0000	H	0.6907	2.6318	0.0000
C	1.2391	0.5065	0.0000	C	-2.1668	2.2663	0.0000	H	3.7764	-2.4748	0.0000
C	0.7653	-0.8215	0.0000	C	-3.3044	1.5021	0.0000	H	5.6406	-0.9111	0.0000
C	-0.6468	-1.1257	0.0000	C	-4.6899	1.8749	0.0000	H	6.4889	1.4268	0.0000
C	-1.5658	-0.0191	0.0000	C	-5.6343	0.9052	0.0000	H	4.9021	3.3314	0.0000
C	-1.0294	1.3514	0.0000	C	-5.2813	-0.4917	0.0000	H	2.4473	2.9304	0.0000
C	0.2955	1.6041	0.0000	C	-3.9895	-0.8998	0.0000	H	-2.1387	-2.6712	0.0000
C	4.9494	-0.0604	0.0000	C	-2.9423	0.0763	0.0000	H	-0.5019	-4.5298	0.0000
C	5.4139	1.2193	0.0000	H	-6.6990	1.1608	0.0000	H	1.9400	-4.0649	0.0000
C	4.5034	2.3114	0.0000	H	-6.0969	-1.2223	0.0000				

Table 3.181: Table of thermodynamic data as a function of temperature for Fluoreno[4,3,2-*de*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.770	543.354	543.354	∞
100	100.916	341.271	735.077	-39.381	566.033	604.700	-315.856
200	196.993	439.053	562.680	-24.725	554.007	648.166	-169.280
250	252.857	488.968	542.924	-13.489	548.367	672.359	-140.479
298.15	307.283	538.170	538.170	0.000	543.354	696.707	-122.058
300	309.348	540.078	538.176	0.570	543.169	697.658	-121.470
350	363.608	591.881	542.144	17.408	538.560	723.781	-108.016
400	413.866	643.766	551.606	36.864	534.569	750.512	-98.005
450	459.344	695.186	564.709	58.715	531.121	777.716	-90.273
500	499.955	745.726	580.292	82.717	528.137	805.297	-84.127
600	567.981	843.140	616.057	136.250	523.295	861.210	-74.973
700	621.733	934.889	655.120	195.838	519.765	917.831	-68.488
800	664.837	1020.825	695.522	260.243	517.395	974.862	-63.651
900	699.977	1101.228	736.183	328.541	516.035	1032.124	-59.902
1000	729.024	1176.529	776.493	400.036	515.550	1089.501	-56.909
1100	753.298	1247.184	816.105	474.187	515.772	1146.899	-54.461
1200	773.759	1313.632	854.825	550.568	516.583	1204.234	-52.418
1300	791.130	1376.270	892.550	628.836	517.828	1261.493	-50.686
1400	805.971	1435.456	929.235	708.710	519.394	1318.647	-49.198
1500	818.721	1491.508	964.868	789.961	521.213	1375.681	-47.904
1600	829.734	1544.708	999.460	872.397	523.172	1432.580	-46.768
1700	839.294	1595.303	1033.033	955.859	525.208	1489.334	-45.761
1800	847.633	1643.518	1065.620	1040.215	527.258	1546.023	-44.863
1900	854.940	1689.547	1097.257	1125.351	529.294	1602.552	-44.056
2000	861.371	1733.566	1127.980	1211.174	531.271	1658.998	-43.328
2100	867.054	1775.733	1157.828	1297.601	533.120	1715.335	-42.666
2200	872.096	1816.187	1186.840	1384.563	534.841	1771.591	-42.062
2300	876.588	1855.054	1215.054	1472.002	536.431	1827.769	-41.509
2400	880.602	1892.448	1242.504	1559.865	537.827	1883.840	-41.000
2500	884.204	1928.470	1269.227	1648.108	539.040	1939.957	-40.532
2600	887.444	1963.214	1295.255	1736.693	540.039	1995.926	-40.098
2700	890.370	1996.762	1320.619	1825.587	540.829	2051.925	-39.696
2800	893.019	2029.191	1345.349	1914.758	541.385	2107.918	-39.323
2900	895.425	2060.571	1369.474	2004.182	541.683	2163.848	-38.974
3000	897.615	2090.965	1393.019	2093.836	541.762	2219.795	-38.649
3100	899.614	2120.430	1416.011	2183.699	541.553	2275.676	-38.344
3200	901.443	2149.021	1438.474	2273.753	541.093	2331.633	-38.059
3300	903.121	2176.786	1460.428	2363.983	540.367	2387.643	-37.792
3400	904.664	2203.770	1481.896	2454.373	539.349	2443.603	-37.541
3500	906.085	2230.015	1502.898	2544.911	538.044	2499.580	-37.303
3600	907.396	2255.559	1523.452	2635.586	536.472	2555.676	-37.081
3700	908.609	2280.437	1543.576	2726.387	534.605	2611.835	-36.872
3800	909.733	2304.684	1563.288	2817.305	532.420	2667.995	-36.673
3900	910.777	2328.328	1582.602	2908.331	529.953	2724.171	-36.485
4000	911.747	2351.399	1601.535	2999.458	527.190	2780.537	-36.309
4100	912.650	2373.924	1620.100	3090.678	524.099	2836.910	-36.142
4200	913.493	2395.927	1638.311	3181.986	520.706	2893.354	-35.983
4300	914.280	2417.431	1656.181	3273.375	516.997	2949.804	-35.832
4400	915.017	2438.458	1673.722	3364.840	512.981	3006.424	-35.690
4500	915.707	2459.029	1690.946	3456.377	508.671	3063.189	-35.556
4600	916.354	2479.163	1707.863	3547.980	504.020	3120.060	-35.429
4700	916.962	2498.877	1724.484	3639.647	499.043	3176.935	-35.307
4800	917.534	2518.188	1740.819	3731.372	493.779	3234.013	-35.193
4900	918.072	2537.112	1756.877	3823.152	488.163	3291.084	-35.083
5000	918.580	2555.665	1772.668	3914.985	482.279	3348.439	-34.980

3.182. Benz[de]indeno[2,1-b]anthracene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 32881-40-6
Point Group: C_s

Length: 15.95 Å
Width: 9.563 Å
Breadth: 3.888 Å
L/B Ratio: 1.668

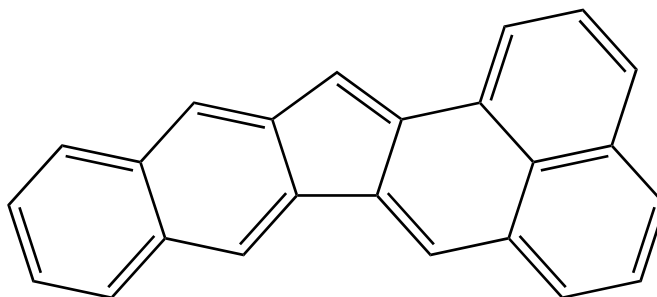
Cartesian coordinates:

C	-0.6754	2.1731	0.0000	C	4.5904	-1.5884	0.0000	H	-5.6956	-2.1663	0.0000
C	-0.5647	0.7898	0.0000	C	5.7183	-0.8021	0.0000	H	-3.3598	2.3167	0.0000
C	0.7284	0.1889	0.0000	C	5.6019	0.5992	0.0000	H	-3.0145	-3.2326	0.0000
C	1.8724	1.0077	0.0000	C	4.3610	1.1920	0.0000	H	-0.1574	-3.1854	0.0000
C	1.7212	2.4106	0.0000	C	-2.8380	-2.1597	0.0000	H	2.2539	-2.8998	0.0000
C	0.4682	2.9803	0.0000	C	-3.7636	-1.1512	0.0000	H	4.6736	-2.6813	0.0000
C	0.8853	-1.2468	0.0000	C	-5.1985	-1.1914	0.0000	H	6.7130	-1.2598	0.0000
C	-0.2928	-2.0972	0.0000	C	-5.8912	-0.0292	0.0000	H	6.5077	1.2146	0.0000
C	-1.5162	-1.5365	0.0000	C	-5.2219	1.2476	0.0000	H	4.2572	2.2880	0.0000
C	-1.7180	-0.0751	0.0000	C	-3.8713	1.3444	0.0000	H	2.6263	3.0370	0.0000
C	3.1872	0.4062	0.0000	C	-3.0771	0.1516	0.0000	H	0.3582	4.0698	0.0000
C	3.3071	-0.9949	0.0000	H	-5.8454	2.1477	0.0000	H	-1.6704	2.6422	0.0000
C	2.1317	-1.8088	0.0000	H	-6.9861	-0.0294	0.0000				

Table 3.182: Table of thermodynamic data as a function of temperature for Benz[de]indeno[2,1-b]anthracene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-45.626	522.690	522.690	∞
100	100.588	341.329	733.694	-39.237	545.514	584.175	-305.135
200	196.216	438.718	561.921	-24.641	533.428	627.655	-163.923
250	251.987	488.448	542.230	-13.445	527.747	651.869	-136.198
298.15	306.356	537.492	537.492	0.000	522.690	676.246	-118.473
300	308.419	539.394	537.498	0.569	522.504	677.197	-117.908
350	362.648	591.051	541.454	17.359	517.847	703.358	-104.968
400	412.898	642.807	550.890	36.767	513.808	730.135	-95.344
450	458.388	694.114	563.960	58.569	510.311	757.389	-87.914
500	499.025	744.555	579.506	82.524	507.281	785.027	-82.009
600	567.129	841.805	615.192	135.968	502.349	841.065	-73.220
700	620.971	933.430	654.179	195.475	498.738	897.826	-66.995
800	664.162	1019.270	694.510	259.808	496.296	955.008	-62.354
900	699.380	1099.598	735.106	328.043	494.873	1012.430	-58.759
1000	728.496	1174.839	775.358	399.481	494.332	1069.972	-55.888
1100	752.830	1245.447	814.917	473.583	494.504	1127.542	-53.541
1200	773.342	1311.856	853.590	549.920	495.271	1185.053	-51.583
1300	790.757	1374.463	891.272	628.148	496.477	1242.491	-49.923
1400	805.636	1433.623	927.918	707.987	498.007	1299.827	-48.496
1500	818.419	1489.653	963.516	789.206	499.794	1357.045	-47.256
1600	829.461	1542.834	998.076	871.613	501.724	1414.131	-46.166
1700	839.046	1593.414	1031.620	955.049	503.735	1471.073	-45.200
1800	847.407	1641.614	1064.180	1039.382	505.761	1527.951	-44.339
1900	854.733	1687.632	1095.792	1124.496	507.776	1584.671	-43.565
2000	861.181	1731.641	1126.492	1210.299	509.732	1641.309	-42.866
2100	866.879	1773.799	1156.319	1296.708	511.563	1697.840	-42.231
2200	871.935	1814.245	1185.312	1383.653	513.268	1754.289	-41.651
2300	876.439	1853.106	1213.507	1471.076	514.842	1810.662	-41.121
2400	880.464	1890.493	1240.941	1558.925	516.224	1866.928	-40.632
2500	884.075	1926.510	1267.648	1647.155	517.424	1923.241	-40.183
2600	887.325	1961.249	1293.661	1735.728	518.411	1979.406	-39.766
2700	890.258	1994.792	1319.011	1824.610	519.188	2035.601	-39.380
2800	892.915	2027.218	1343.728	1913.771	519.734	2091.792	-39.022
2900	895.327	2058.594	1367.841	2003.185	520.022	2147.919	-38.687
3000	897.523	2088.985	1391.375	2092.829	520.091	2204.064	-38.375
3100	899.527	2118.447	1414.356	2182.683	519.873	2260.143	-38.082
3200	901.362	2147.036	1436.808	2272.729	519.405	2316.299	-37.809
3300	903.044	2174.798	1458.753	2362.950	518.670	2372.507	-37.553
3400	904.591	2201.780	1480.212	2453.333	517.645	2428.666	-37.311
3500	906.015	2228.023	1501.204	2543.864	516.333	2484.843	-37.083
3600	907.331	2253.565	1521.750	2634.532	514.755	2541.138	-36.870
3700	908.547	2278.441	1541.867	2725.327	512.881	2597.497	-36.669
3800	909.674	2302.686	1561.570	2816.239	510.690	2653.856	-36.479
3900	910.720	2326.329	1580.878	2907.259	508.217	2710.232	-36.299
4000	911.693	2349.399	1599.804	2998.380	505.449	2766.798	-36.130
4100	912.599	2371.922	1618.362	3089.595	502.353	2823.371	-35.969
4200	913.444	2393.924	1636.567	3180.898	498.954	2880.016	-35.817
4300	914.234	2415.427	1654.431	3272.282	495.241	2936.665	-35.673
4400	914.972	2436.453	1671.966	3363.743	491.220	2993.486	-35.536
4500	915.664	2457.023	1689.184	3455.275	486.906	3050.452	-35.408
4600	916.313	2477.156	1706.096	3546.875	482.251	3107.524	-35.286
4700	916.923	2496.869	1722.712	3638.537	477.269	3164.599	-35.170
4800	917.496	2516.179	1739.042	3730.258	472.001	3221.878	-35.060
4900	918.036	2535.103	1755.096	3822.035	466.382	3279.150	-34.955
5000	918.545	2553.655	1770.882	3913.864	460.494	3336.706	-34.858

3.183. Benz[5,6]indeno[2,1-*a*]phenalene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 76727-41-8
Point Group: C_s

Length: 15.83 Å
Width: 9.187 Å
Breadth: 3.885 Å
L/B Ratio: 1.723

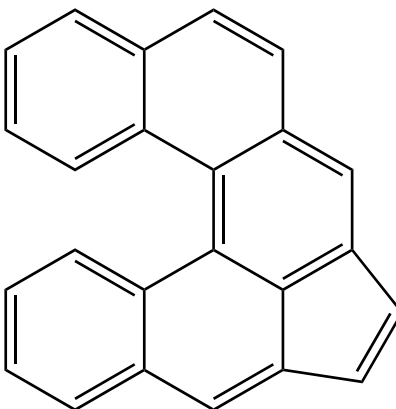
Cartesian coordinates:

C	2.7063	2.3827	0.0000	C	-0.3296	1.8343	0.0000	H	-4.4714	-2.8105	0.0000
C	2.1298	1.1313	0.0000	C	-1.5964	1.0983	0.0000	H	-5.5191	2.0669	0.0000
C	2.9580	-0.0370	0.0000	C	-2.8850	1.5422	0.0000	H	-2.0626	-2.3225	0.0000
C	4.3598	0.1161	0.0000	C	-3.9383	0.5779	0.0000	H	-3.1249	2.6107	0.0000
C	4.9220	1.4220	0.0000	C	-3.6420	-0.8036	0.0000	H	-0.2667	2.9217	0.0000
C	4.1107	2.5243	0.0000	C	-2.2848	-1.2497	0.0000	H	0.5456	-2.5415	0.0000
C	2.4004	-1.3533	0.0000	C	-1.2950	-0.3149	0.0000	H	2.8149	-3.4645	0.0000
C	0.9561	-1.5251	0.0000	C	-4.7073	-1.7402	0.0000	H	5.2741	-3.1777	0.0000
C	0.1638	-0.4408	0.0000	C	-6.0091	-1.3114	0.0000	H	6.2778	-0.9046	0.0000
C	0.6962	0.9381	0.0000	C	-6.3055	0.0687	0.0000	H	6.0128	1.5280	0.0000
C	5.1896	-1.0352	0.0000	C	-5.2947	0.9942	0.0000	H	4.5417	3.5310	0.0000
C	4.6347	-2.2887	0.0000	H	-7.3523	0.3896	0.0000	H	2.0775	3.2806	0.0000
C	3.2355	-2.4523	0.0000	H	-6.8318	-2.0339	0.0000				

Table 3.183: Table of thermodynamic data as a function of temperature for Benz[5,6]indeno[2,1-*a*]phenalene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.015	447.948	447.948	∞
100	98.618	337.462	725.470	-38.801	471.208	510.255	-266.524
200	193.957	433.418	555.485	-24.413	458.913	554.200	-144.739
250	249.653	482.634	535.969	-13.334	453.117	578.692	-120.909
298.15	304.058	531.269	531.269	0.000	447.948	603.360	-105.704
300	306.124	533.156	531.275	0.564	447.758	604.322	-105.220
350	360.446	584.466	535.203	17.242	442.989	630.805	-94.140
400	410.815	635.936	544.579	36.543	438.842	657.917	-85.913
450	456.438	687.005	557.573	58.244	435.245	685.522	-79.572
500	497.218	737.247	573.037	82.105	432.120	713.520	-74.539
600	565.619	834.194	608.556	135.383	427.022	770.304	-67.060
700	619.749	925.608	647.388	194.754	423.275	827.838	-61.773
800	663.198	1011.303	687.580	258.978	420.724	885.810	-57.836
900	698.634	1091.530	728.055	327.127	419.216	944.034	-54.789
1000	727.926	1166.702	768.202	398.500	418.609	1002.387	-52.358
1100	752.398	1237.263	807.670	472.552	418.732	1060.773	-50.371
1200	773.018	1303.639	846.262	548.852	419.462	1119.104	-48.712
1300	790.517	1366.223	883.875	627.052	420.639	1177.365	-47.306
1400	805.459	1425.368	920.461	706.870	422.149	1235.525	-46.097
1500	818.291	1481.387	956.005	788.074	423.920	1293.570	-45.045
1600	829.370	1534.561	990.517	870.470	425.840	1351.483	-44.120
1700	838.983	1585.136	1024.019	953.899	427.842	1409.252	-43.300
1800	847.366	1633.334	1056.542	1038.226	429.863	1466.958	-42.569
1900	854.708	1679.350	1088.120	1123.337	431.875	1524.506	-41.911
2000	861.169	1723.358	1118.789	1209.138	433.829	1581.973	-41.316
2100	866.877	1765.516	1148.589	1295.546	435.660	1639.332	-40.775
2200	871.940	1805.962	1177.557	1382.492	437.364	1696.609	-40.282
2300	876.449	1844.823	1205.729	1469.916	438.939	1753.811	-39.829
2400	880.478	1882.211	1233.142	1557.766	440.322	1810.905	-39.413
2500	884.092	1918.228	1259.829	1645.997	441.524	1868.046	-39.030
2600	887.344	1952.967	1285.824	1734.572	442.512	1925.039	-38.674
2700	890.279	1986.512	1311.158	1823.456	443.292	1982.063	-38.345
2800	892.937	2018.938	1335.860	1912.619	443.840	2039.081	-38.039
2900	895.349	2050.315	1359.958	2002.035	444.130	2096.036	-37.753
3000	897.546	2080.707	1383.480	2091.681	444.202	2153.009	-37.486
3100	899.551	2110.170	1406.448	2181.538	443.986	2209.916	-37.236
3200	901.385	2138.759	1428.889	2271.586	443.520	2266.899	-37.003
3300	903.067	2166.522	1450.822	2361.810	442.788	2323.935	-36.784
3400	904.614	2193.505	1472.271	2452.195	441.765	2380.922	-36.578
3500	906.038	2219.748	1493.254	2542.728	440.456	2437.926	-36.383
3600	907.353	2245.291	1513.791	2633.399	438.879	2495.049	-36.201
3700	908.569	2270.168	1533.899	2724.196	437.008	2552.235	-36.030
3800	909.695	2294.413	1553.595	2815.109	434.819	2609.421	-35.868
3900	910.741	2318.057	1572.895	2906.132	432.348	2666.625	-35.715
4000	911.713	2341.127	1591.813	2997.255	429.582	2724.018	-35.571
4100	912.619	2363.651	1610.365	3088.472	426.488	2781.418	-35.435
4200	913.463	2385.653	1628.563	3179.777	423.091	2838.889	-35.306
4300	914.252	2407.157	1646.421	3271.163	419.380	2896.366	-35.183
4400	914.990	2428.183	1663.950	3362.626	415.361	2954.014	-35.068
4500	915.682	2448.754	1681.163	3454.160	411.048	3011.807	-34.959
4600	916.330	2468.887	1698.069	3545.761	406.395	3069.705	-34.857
4700	916.940	2488.600	1714.680	3637.424	401.415	3127.608	-34.759
4800	917.512	2507.911	1731.005	3729.147	396.149	3185.714	-34.667
4900	918.052	2526.835	1747.054	3820.926	390.531	3243.812	-34.579
5000	918.560	2545.387	1762.836	3912.757	384.645	3302.195	-34.497

3.184. Naphth[1,2-*a*]acephenanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 777080-18-9
Point Group: C₁

Length: 12.93 Å
Width: 11.61 Å
Breadth: 5.672 Å
L/B Ratio: 1.114

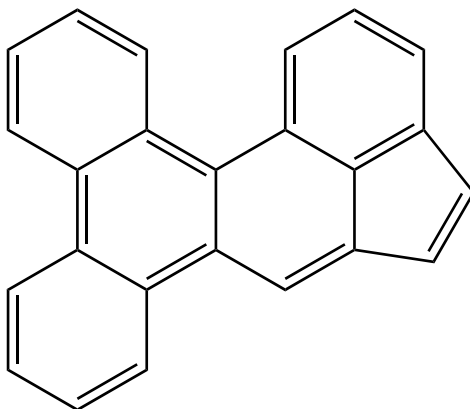
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C	4.2179	-0.3072	-0.5850	C	0.1357	-2.2752	0.3590	H	-4.0328	1.2338	-1.6604
C	3.0456	0.5699	-0.4335	C	1.5182	-2.6287	0.2404	H	-5.6022	-0.4673	-0.7558
C	1.9294	-0.3012	-0.1677	C	0.6228	0.1004	0.0279	H	-4.7090	-2.4838	0.3981
C	2.4007	-1.6509	-0.1029	C	2.8405	1.9082	-0.4693	H	-2.8249	-3.8502	1.0895
C	-2.2868	0.2723	-0.8676	C	0.4562	1.5324	0.1982	H	-0.3782	-4.2808	1.0358
C	-3.6383	0.3856	-1.0913	C	1.5327	2.4012	-0.1135	H	1.8308	-3.6663	0.3995
C	-4.5254	-0.5886	-0.5999	C	1.3554	3.7986	0.0089	H	3.6393	2.6187	-0.7069
C	-4.0329	-1.6964	0.0459	C	0.1851	4.3184	0.5086	H	2.1744	4.4657	-0.2848
C	-1.7566	-0.8197	-0.1390	C	-0.8377	3.4541	0.9308	H	0.0528	5.4011	0.6027
C	-2.6409	-1.8482	0.2427	C	-0.7013	2.0932	0.7822	H	-1.7432	3.8704	1.3846
C	-2.1214	-3.0822	0.7490	H	4.4792	-2.4824	-0.4086	H	-1.5993	1.0239	-1.2783
C	-0.7847	-3.3073	0.7371	H	5.2139	0.0636	-0.8189				

Table 3.184: Table of thermodynamic data as a function of temperature for Naphth[1,2-*a*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.757	496.921	496.921	∞
100	97.438	331.084	718.110	-38.703	520.278	559.963	-292.489
200	193.462	426.446	548.431	-24.397	507.902	604.583	-157.898
250	249.493	475.587	528.923	-13.334	502.089	629.426	-131.509
298.15	304.220	524.222	524.222	0.000	496.921	654.433	-114.652
300	306.298	526.110	524.227	0.565	496.731	655.409	-114.114
350	360.906	577.469	528.159	17.259	491.978	682.242	-101.817
400	411.489	629.015	537.546	36.588	487.860	709.703	-92.676
450	457.249	680.172	550.557	58.327	484.300	737.651	-85.623
500	498.100	730.504	566.043	82.231	481.217	765.989	-80.021
600	566.504	827.615	601.619	135.598	476.210	823.439	-71.685
700	620.534	919.158	640.511	195.053	472.547	881.624	-65.786
800	663.850	1004.949	680.763	259.349	470.067	940.236	-61.390
900	699.153	1085.246	721.294	327.557	468.617	999.091	-57.985
1000	728.329	1160.466	761.490	398.976	468.056	1058.070	-55.267
1100	752.705	1231.060	801.003	473.063	468.215	1117.078	-53.045
1200	773.249	1297.460	839.636	549.389	468.971	1176.028	-51.190
1300	790.687	1360.060	877.284	627.609	470.168	1234.906	-49.618
1400	805.583	1419.216	913.900	707.442	471.693	1293.682	-48.267
1500	818.379	1475.242	949.472	788.656	473.475	1352.342	-47.092
1600	829.431	1528.421	984.008	871.060	475.402	1410.869	-46.059
1700	839.023	1578.999	1017.532	954.494	477.409	1469.252	-45.144
1800	847.390	1627.199	1050.074	1038.824	479.433	1527.572	-44.328
1900	854.721	1673.215	1081.670	1123.937	481.447	1585.734	-43.594
2000	861.172	1717.224	1112.355	1209.738	483.402	1643.814	-42.931
2100	866.872	1759.382	1142.169	1296.146	485.232	1701.786	-42.329
2200	871.931	1799.828	1171.150	1383.091	486.936	1759.676	-41.779
2300	876.435	1838.688	1199.334	1470.514	488.510	1817.492	-41.276
2400	880.462	1876.075	1226.758	1558.363	489.891	1875.200	-40.812
2500	884.074	1912.092	1253.455	1646.593	491.092	1932.954	-40.386
2600	887.324	1946.830	1279.459	1735.165	492.078	1990.561	-39.990
2700	890.259	1980.374	1304.801	1824.047	492.856	2048.198	-39.624
2800	892.915	2012.800	1329.511	1913.208	493.402	2105.830	-39.284
2900	895.328	2044.176	1353.617	2002.622	493.690	2163.399	-38.966
3000	897.524	2074.567	1377.145	2092.266	493.759	2220.986	-38.670
3100	899.529	2104.030	1400.120	2182.120	493.541	2278.507	-38.392
3200	901.364	2132.618	1422.566	2272.166	493.073	2336.104	-38.132
3300	903.046	2160.380	1444.505	2362.388	492.339	2393.755	-37.889
3400	904.593	2187.362	1465.959	2452.771	491.314	2451.355	-37.660
3500	906.018	2213.605	1486.947	2543.303	490.002	2508.974	-37.444
3600	907.333	2239.147	1507.488	2633.971	488.424	2566.711	-37.241
3700	908.549	2264.024	1527.601	2724.766	486.551	2624.511	-37.051
3800	909.676	2288.268	1547.301	2815.678	484.360	2682.312	-36.870
3900	910.723	2311.911	1566.604	2906.698	481.887	2740.130	-36.699
4000	911.695	2334.981	1585.526	2997.820	479.119	2798.138	-36.539
4100	912.601	2357.505	1604.081	3089.035	476.023	2856.152	-36.387
4200	913.446	2379.506	1622.283	3180.338	472.625	2914.239	-36.243
4300	914.236	2401.010	1640.144	3271.723	468.912	2972.330	-36.106
4400	914.974	2422.036	1657.676	3363.184	464.892	3030.593	-35.977
4500	915.666	2442.606	1674.891	3454.716	460.577	3089.000	-35.855
4600	916.315	2462.738	1691.800	3546.316	455.922	3147.514	-35.740
4700	916.925	2482.452	1708.414	3637.978	450.941	3206.031	-35.630
4800	917.498	2501.762	1724.741	3729.699	445.673	3264.752	-35.527
4900	918.038	2520.686	1740.793	3821.476	440.054	3323.465	-35.428
5000	918.547	2539.238	1756.577	3913.306	434.167	3382.463	-35.336

3.185. Indeno[7,1-*ab*]triphenylene



Other names: Benzo[*g*]cyclopenta[*qr*]chrysene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 908068-12-2

Point Group: C₁

Length: 13.50 Å

Width: 11.05 Å

Breadth: 4.791 Å

L/B Ratio: 1.222

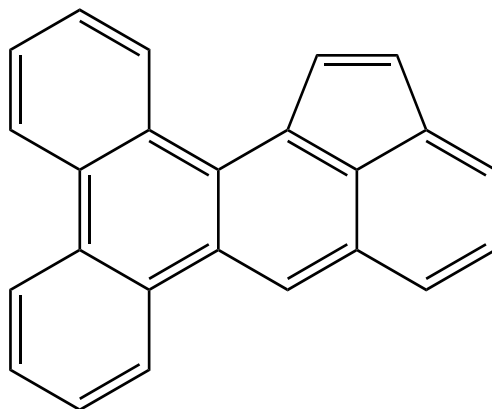
Cartesian coordinates:

C	4.4496	-1.5738	0.1749	C	-2.2106	0.9652	-0.0280	H	5.5320	1.1512	-0.4533
C	3.4180	-2.4394	0.3717	C	-3.2274	1.9411	-0.0231	H	1.5539	2.8190	-0.6585
C	2.1463	-1.7038	0.2797	C	-2.9367	3.2691	0.1984	H	3.9765	3.0495	-0.8431
C	2.4949	-0.3363	0.0460	C	-1.6143	3.6493	0.4505	H	0.5073	-3.0775	0.4200
C	3.9136	-0.2222	-0.0575	C	-0.6063	2.7094	0.4168	H	-4.2683	1.6225	-0.1862
C	4.4529	0.9986	-0.3591	C	-2.5531	-0.4395	-0.1261	H	-3.7328	4.0205	0.1972
C	2.1890	1.9459	-0.4571	C	-1.5482	-1.4072	0.0294	H	-1.3835	4.6951	0.6788
C	3.5550	2.0756	-0.5699	C	-1.9188	-2.7689	0.0224	H	0.4188	3.0327	0.6424
C	1.5873	0.7028	-0.1061	C	-3.2296	-3.1522	-0.1612	H	-1.1466	-3.5398	0.1608
C	0.8293	-2.0339	0.2949	C	-4.2237	-2.1836	-0.3467	H	-3.4979	-4.2137	-0.1664
C	0.1915	0.3569	0.0487	C	-3.8874	-0.8480	-0.3260	H	-5.2626	-2.4912	-0.5026
C	-0.1556	-1.0000	0.1379	H	5.5135	-1.8022	0.1788	H	-4.6630	-0.0788	-0.4596
C	-0.8660	1.3540	0.1251	H	3.4790	-3.5085	0.5643				

Table 3.185: Table of thermodynamic data as a function of temperature for Indeno[7,1-*ab*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.087	490.285	490.285	∞
100	99.428	338.039	726.001	-38.796	513.548	552.538	-288.610
200	193.769	434.237	556.137	-24.380	501.283	596.406	-155.762
250	249.279	483.386	536.648	-13.315	495.471	620.859	-129.719
298.15	303.697	531.954	531.954	0.000	490.285	645.491	-113.085
300	305.766	533.839	531.960	0.564	490.093	646.453	-112.555
350	360.207	585.103	535.884	17.226	485.309	672.902	-100.423
400	410.721	636.549	545.253	36.518	481.154	699.984	-91.407
450	456.466	687.615	558.240	58.219	477.555	727.558	-84.451
500	497.330	737.865	573.698	82.083	474.434	755.525	-78.928
600	565.781	834.839	609.213	135.376	469.352	812.247	-70.711
700	619.853	926.275	648.045	194.761	465.619	869.714	-64.898
800	663.199	1011.977	688.239	258.990	463.073	927.620	-60.566
900	698.526	1092.198	728.715	327.134	461.559	985.776	-57.212
1000	727.726	1167.354	768.862	398.492	460.937	1044.063	-54.535
1100	752.127	1237.891	808.328	472.520	461.036	1102.385	-52.347
1200	772.698	1304.242	846.917	548.790	461.735	1160.654	-50.521
1300	790.164	1366.799	884.525	626.956	462.879	1218.856	-48.973
1400	805.089	1425.917	921.104	706.738	464.353	1276.960	-47.643
1500	817.914	1481.911	956.641	787.904	466.087	1334.952	-46.486
1600	828.994	1535.060	991.146	870.263	467.969	1392.813	-45.470
1700	838.614	1585.613	1024.640	953.654	469.934	1450.534	-44.569
1800	847.007	1633.790	1057.154	1037.945	471.919	1508.194	-43.766
1900	854.362	1679.786	1088.722	1123.021	473.895	1565.697	-43.043
2000	860.836	1723.777	1119.383	1208.788	475.816	1623.121	-42.391
2100	866.558	1765.919	1149.175	1295.163	477.613	1680.439	-41.798
2200	871.635	1806.351	1178.133	1382.078	479.287	1737.676	-41.257
2300	876.159	1845.198	1206.297	1469.472	480.832	1794.840	-40.761
2400	880.202	1882.574	1233.702	1557.294	482.186	1851.897	-40.305
2500	883.830	1918.581	1260.381	1645.499	483.361	1909.002	-39.886
2600	887.094	1953.310	1286.368	1734.048	484.324	1965.961	-39.496
2700	890.042	1986.845	1311.695	1822.907	485.080	2022.950	-39.136
2800	892.711	2019.263	1336.389	1912.047	485.604	2079.936	-38.801
2900	895.135	2050.632	1360.480	2001.441	485.873	2136.859	-38.488
3000	897.341	2081.017	1383.994	2091.066	485.923	2193.800	-38.197
3100	899.356	2110.474	1406.957	2180.903	485.687	2250.677	-37.923
3200	901.200	2139.056	1429.390	2270.932	485.203	2307.630	-37.667
3300	902.891	2166.814	1451.318	2361.138	484.452	2364.637	-37.428
3400	904.445	2193.792	1472.760	2451.505	483.412	2421.594	-37.202
3500	905.877	2220.030	1493.738	2542.023	482.086	2478.570	-36.990
3600	907.199	2245.568	1514.269	2632.677	480.494	2535.665	-36.791
3700	908.422	2270.441	1534.371	2723.459	478.608	2592.823	-36.603
3800	909.555	2294.683	1554.062	2814.359	476.404	2649.983	-36.426
3900	910.607	2318.323	1573.357	2905.367	473.920	2707.159	-36.258
4000	911.585	2341.390	1592.270	2996.478	471.140	2764.526	-36.100
4100	912.495	2363.910	1610.817	3087.682	468.034	2821.900	-35.951
4200	913.345	2385.910	1629.011	3178.975	464.625	2879.346	-35.809
4300	914.139	2407.410	1646.864	3270.349	460.902	2936.797	-35.674
4400	914.881	2428.435	1664.389	3361.801	456.872	2994.420	-35.548
4500	915.577	2449.003	1681.597	3453.324	452.549	3052.187	-35.428
4600	916.230	2469.133	1698.500	3544.915	447.885	3110.061	-35.315
4700	916.843	2488.844	1715.106	3636.568	442.895	3167.939	-35.207
4800	917.419	2508.153	1731.428	3728.282	437.620	3226.020	-35.106
4900	917.962	2527.075	1747.473	3820.051	431.993	3284.095	-35.008
5000	918.473	2545.626	1763.251	3911.873	426.098	3342.454	-34.918

3.186. Indeno[1,7-*ab*]triphenylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-20-2
Point Group: C₁

Length: 13.74 Å
Width: 11.16 Å
Breadth: 4.366 Å
L/B Ratio: 1.231

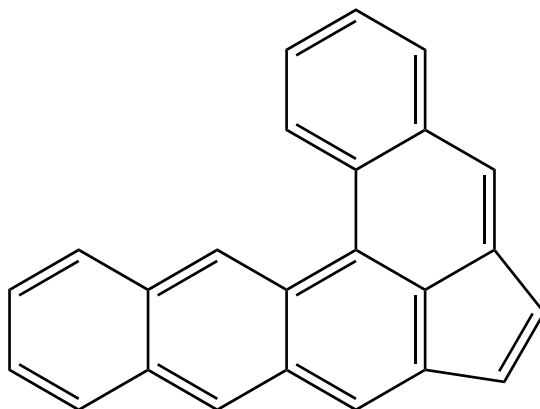
Cartesian coordinates:

C	-3.8172	1.1843	0.1955	C	1.4177	-0.9742	0.0834	H	5.8853	-0.3827	0.1453
C	-2.5330	0.6267	0.0734	C	3.5395	2.1000	-0.1971	H	5.6750	2.0700	-0.1511
C	-1.4202	1.4753	-0.0347	C	4.7570	1.4740	-0.1008	H	3.4722	3.1861	-0.3212
C	-1.6326	2.8656	-0.0485	C	4.8896	0.0642	0.0675	H	0.8338	2.8855	-0.2539
C	-2.9025	3.3998	0.0615	C	3.7530	-0.6899	0.1274	H	-4.4778	-1.2233	0.1242
C	-4.0040	2.5533	0.1922	C	-3.4741	-1.6645	0.0284	H	-4.2189	-3.6816	-0.0867
C	-0.0670	0.9218	-0.0939	C	-3.3365	-3.0339	-0.0946	H	-1.9466	-4.6645	-0.3705
C	0.1151	-0.5079	-0.0219	C	-2.0641	-3.5833	-0.2440	H	0.0354	-3.2236	-0.3736
C	-1.0622	-1.3716	-0.0670	C	-0.9509	-2.7624	-0.2339	H	-0.7720	3.5441	-0.1446
C	-2.3530	-0.8180	0.0251	C	3.4392	-2.1145	0.2975	H	-3.0452	4.4853	0.0499
C	1.0060	1.8012	-0.1743	C	2.0880	-2.2782	0.2745	H	-5.0103	2.9733	0.2886
C	2.3370	1.3356	-0.1336	H	4.1943	-2.8872	0.4264	H	-4.6850	0.5142	0.2903
C	2.4855	-0.0348	0.0165	H	1.5554	-3.2230	0.3945				

Table 3.186: Table of thermodynamic data as a function of temperature for Indeno[1,7-*ab*]triphenylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-45.146	490.212	490.212	∞
100	99.422	339.574	727.776	-38.820	513.452	552.288	-288.480
200	193.905	435.806	557.797	-24.398	501.192	596.001	-155.656
250	249.471	484.992	538.294	-13.325	495.389	620.374	-129.617
298.15	303.912	533.596	533.596	0.000	490.212	644.929	-112.987
300	305.981	535.483	533.602	0.564	490.021	645.888	-112.457
350	360.424	586.780	537.529	17.238	485.247	672.254	-100.326
400	410.928	638.255	546.904	36.540	481.103	699.251	-91.311
450	456.661	689.344	559.898	58.251	477.514	726.739	-84.356
500	497.512	739.614	575.364	82.125	474.403	754.619	-78.833
600	565.939	836.619	610.895	135.434	469.337	811.164	-70.617
700	619.992	928.077	649.743	194.834	465.619	868.453	-64.803
800	663.323	1013.797	689.951	259.076	463.086	926.177	-60.472
900	698.639	1094.032	730.441	327.232	461.584	984.150	-57.117
1000	727.828	1169.199	770.598	398.601	460.972	1042.253	-54.441
1100	752.221	1239.746	810.075	472.639	461.081	1100.390	-52.252
1200	772.784	1306.105	848.673	548.917	461.790	1158.474	-50.426
1300	790.243	1368.668	886.290	627.092	462.942	1216.489	-48.878
1400	805.161	1427.792	922.877	706.881	464.423	1274.406	-47.548
1500	817.981	1483.790	958.421	788.055	466.164	1332.210	-46.391
1600	829.056	1536.944	992.931	870.420	468.052	1389.883	-45.374
1700	838.671	1587.500	1026.431	953.817	470.024	1447.415	-44.473
1800	847.059	1635.680	1058.951	1038.113	472.014	1504.886	-43.670
1900	854.410	1681.679	1090.525	1123.194	473.995	1562.200	-42.947
2000	860.880	1725.673	1121.190	1208.966	475.920	1619.435	-42.294
2100	866.599	1767.817	1150.986	1295.345	477.722	1676.563	-41.701
2200	871.674	1808.250	1179.948	1382.264	479.400	1733.610	-41.160
2300	876.195	1847.099	1208.116	1469.662	480.949	1790.584	-40.665
2400	880.236	1884.477	1235.524	1557.487	482.307	1847.451	-40.208
2500	883.861	1920.485	1262.207	1645.695	483.485	1904.366	-39.789
2600	887.124	1955.215	1288.197	1734.247	484.451	1961.134	-39.399
2700	890.069	1988.751	1313.526	1823.109	485.209	2017.933	-39.038
2800	892.737	2021.170	1338.223	1912.252	485.737	2074.728	-38.704
2900	895.159	2052.540	1362.317	2001.648	486.007	2131.460	-38.391
3000	897.365	2082.925	1385.833	2091.276	486.060	2188.211	-38.099
3100	899.378	2112.383	1408.798	2181.115	485.827	2244.896	-37.825
3200	901.220	2140.967	1431.234	2271.146	485.344	2301.658	-37.570
3300	902.910	2168.725	1453.163	2361.354	484.596	2358.474	-37.331
3400	904.464	2195.703	1474.608	2451.724	483.557	2415.240	-37.105
3500	905.895	2221.942	1495.587	2542.243	482.233	2472.025	-36.892
3600	907.216	2247.481	1516.120	2632.899	480.643	2528.928	-36.693
3700	908.438	2272.354	1536.224	2723.682	478.758	2585.896	-36.506
3800	909.570	2296.596	1555.916	2814.584	476.556	2642.864	-36.328
3900	910.621	2320.236	1575.212	2905.594	474.074	2699.849	-36.160
4000	911.598	2343.304	1594.127	2996.705	471.295	2757.024	-36.002
4100	912.508	2365.825	1612.676	3087.911	468.190	2814.207	-35.853
4200	913.358	2387.824	1630.871	3179.205	464.783	2871.461	-35.711
4300	914.151	2409.325	1648.725	3270.581	461.061	2928.721	-35.576
4400	914.893	2430.350	1666.251	3362.033	457.032	2986.152	-35.449
4500	915.588	2450.918	1683.461	3453.558	452.710	3043.728	-35.330
4600	916.240	2471.049	1700.364	3545.150	448.047	3101.410	-35.217
4700	916.853	2490.760	1716.972	3636.804	443.058	3159.097	-35.109
4800	917.429	2510.069	1733.295	3728.519	437.784	3216.987	-35.007
4900	917.971	2528.992	1749.341	3820.289	432.158	3274.870	-34.910
5000	918.482	2547.542	1765.120	3912.112	426.264	3333.037	-34.819

3.187. Dibenz[*a,k*]acephenanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 777080-19-0
Point Group: C₁

Length: 14.15 Å
Width: 11.31 Å
Breadth: 4.474 Å
L/B Ratio: 1.252

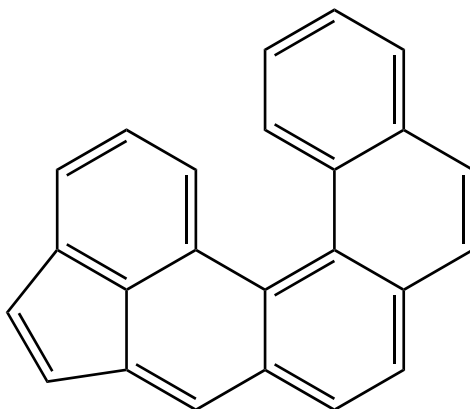
Cartesian coordinates:

C	-1.6036	1.2662	-0.0229	C	0.5410	0.2073	0.0222	H	5.6950	-2.5202	-0.4089
C	-1.0230	2.5884	0.0581	C	1.1223	1.5146	0.1677	H	6.6742	-0.2886	0.0273
C	-2.1436	3.5377	-0.0267	C	0.3127	2.7154	0.1966	H	5.2031	1.6936	0.3414
C	-3.3079	2.8506	-0.1596	C	-0.9143	0.0778	0.0249	H	3.2296	-2.8169	-0.5183
C	-3.0271	1.4065	-0.1526	C	-3.7945	0.2919	-0.2429	H	2.9393	2.6624	0.3612
C	5.0223	-1.6679	-0.2677	C	-1.7435	-1.1100	0.0683	H	1.0073	-1.8668	-0.3922
C	5.5847	-0.3862	-0.0203	C	-3.1463	-0.9840	-0.1175	H	0.8016	3.6898	0.3033
C	4.7801	0.7004	0.1531	C	-3.9622	-2.1421	-0.1351	H	-4.8799	0.3395	-0.3814
C	3.6702	-1.8317	-0.3279	C	-3.4260	-3.3860	0.0817	H	-5.0376	-2.0290	-0.3164
C	2.7987	-0.7149	-0.1408	C	-2.0525	-3.5104	0.3520	H	-4.0587	-4.2791	0.0637
C	3.3600	0.5615	0.0905	C	-1.2407	-2.4025	0.3514	H	-1.6354	-4.4991	0.5705
C	2.5031	1.6644	0.2247	H	-2.0136	4.6175	0.0121	H	-0.1807	-2.5317	0.6053
C	1.4018	-0.8636	-0.1786	H	-4.3113	3.2617	-0.2534				

Table 3.187: Table of thermodynamic data as a function of temperature for Dibenz[*a,k*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.831	478.440	478.440	∞
100	97.762	333.938	721.196	-38.726	501.774	541.174	-282.675
200	193.576	429.485	551.459	-24.395	489.423	585.497	-152.913
250	249.466	478.636	531.954	-13.329	483.613	610.188	-127.489
298.15	304.069	527.255	527.255	0.000	478.440	635.048	-111.255
300	306.142	529.142	527.261	0.564	478.250	636.018	-110.738
350	360.635	580.469	531.190	17.248	473.486	662.701	-98.901
400	411.125	631.972	540.570	36.561	469.352	690.013	-90.105
450	456.818	683.082	553.571	58.280	465.772	717.814	-83.320
500	497.628	733.366	569.045	82.161	462.667	746.007	-77.933
600	566.005	830.387	604.589	135.479	457.610	803.176	-69.921
700	620.053	921.855	643.448	194.885	453.898	861.087	-64.254
800	663.404	1007.583	683.666	259.134	451.372	919.433	-60.032
900	698.748	1087.830	724.164	327.300	449.880	978.028	-56.762
1000	727.965	1163.010	764.330	398.680	449.280	1036.750	-54.153
1100	752.378	1233.571	803.814	472.733	449.404	1095.505	-52.020
1200	772.956	1299.944	842.420	549.028	450.129	1154.205	-50.240
1300	790.424	1362.522	880.044	627.220	451.299	1212.836	-48.731
1400	805.345	1421.659	916.639	707.028	452.798	1271.367	-47.434
1500	818.164	1477.670	952.190	788.219	454.558	1329.784	-46.306
1600	829.236	1530.835	986.708	870.603	456.464	1388.069	-45.315
1700	838.846	1581.402	1020.215	954.018	458.453	1446.210	-44.436
1800	847.228	1629.592	1052.741	1038.331	460.460	1504.291	-43.652
1900	854.573	1675.600	1084.322	1123.429	462.458	1562.214	-42.947
2000	861.036	1719.602	1114.994	1209.216	464.399	1620.055	-42.311
2100	866.747	1761.753	1144.795	1295.611	466.216	1677.790	-41.732
2200	871.815	1802.193	1173.764	1382.544	467.908	1735.444	-41.204
2300	876.329	1841.049	1201.937	1469.956	469.471	1793.023	-40.720
2400	880.363	1878.432	1229.351	1557.794	470.842	1850.495	-40.274
2500	883.982	1914.445	1256.039	1646.015	472.033	1908.014	-39.865
2600	887.238	1949.179	1282.034	1734.578	473.010	1965.386	-39.484
2700	890.178	1982.720	1307.368	1823.452	473.780	2022.788	-39.132
2800	892.840	2015.143	1332.070	1912.605	474.318	2080.186	-38.806
2900	895.257	2046.517	1356.168	2002.012	474.599	2137.521	-38.500
3000	897.458	2076.905	1379.689	2091.649	474.661	2194.874	-38.215
3100	899.467	2106.366	1402.657	2181.497	474.437	2252.161	-37.948
3200	901.305	2134.952	1425.097	2271.537	473.963	2309.525	-37.698
3300	902.991	2162.713	1447.030	2361.753	473.223	2366.942	-37.465
3400	904.540	2189.693	1468.478	2452.130	472.192	2424.309	-37.244
3500	905.968	2215.934	1489.461	2542.657	470.876	2481.695	-37.037
3600	907.286	2241.475	1509.997	2633.320	469.292	2539.199	-36.842
3700	908.505	2266.350	1530.104	2724.111	467.415	2596.767	-36.659
3800	909.634	2290.594	1549.800	2815.018	465.219	2654.335	-36.486
3900	910.682	2314.236	1569.099	2906.035	462.743	2711.920	-36.321
4000	911.657	2337.305	1588.017	2997.152	459.970	2769.695	-36.168
4100	912.565	2359.827	1606.568	3088.364	456.871	2827.478	-36.022
4200	913.411	2381.828	1624.765	3179.663	453.469	2885.332	-35.884
4300	914.202	2403.330	1642.622	3271.044	449.752	2943.191	-35.752
4400	914.942	2424.356	1660.151	3362.502	445.729	3001.222	-35.628
4500	915.636	2444.925	1677.363	3454.031	441.411	3059.397	-35.512
4600	916.286	2465.057	1694.269	3545.627	436.754	3117.679	-35.402
4700	916.897	2484.770	1710.879	3637.287	431.769	3175.965	-35.296
4800	917.471	2504.079	1727.203	3729.006	426.499	3234.453	-35.197
4900	918.012	2523.003	1743.252	3820.780	420.877	3292.935	-35.102
5000	918.522	2541.554	1759.033	3912.607	414.987	3351.701	-35.014

3.188. Naphth[2,1-*l*]acephenanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-27-9
Point Group: C₁

Length: 13.25 Å
Width: 10.12 Å
Breadth: 5.983 Å
L/B Ratio: 1.309

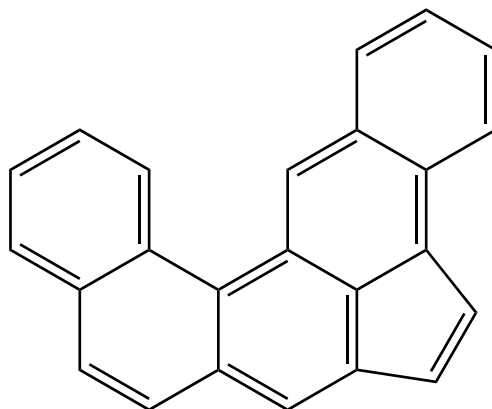
Cartesian coordinates:

C	-3.9257	0.8750	0.6658	C	1.6761	-2.6098	1.1091	H	3.7471	-3.2795	0.9445
C	-3.3579	-0.3392	0.1593	C	4.7186	-0.6876	-0.2101	H	-0.5105	-1.5149	-1.3108
C	-1.9966	-0.3823	-0.2024	C	4.5227	0.6031	-0.5952	H	1.3617	-3.5456	1.5846
C	-1.1575	0.7702	0.0534	C	3.0968	0.9407	-0.4538	H	2.7873	3.0369	-0.8118
C	-1.8050	1.9892	0.3057	C	0.9399	1.9870	-0.2539	H	0.7454	4.1516	-0.3709
C	-3.1906	2.0135	0.6712	C	2.3514	2.0687	-0.5420	H	-1.6342	4.1568	0.3439
C	-1.5384	-1.5095	-0.9245	C	0.2170	3.2104	-0.1792	H	-3.6330	2.9706	0.9704
C	0.7376	-1.6220	0.8908	C	-1.0970	3.2149	0.1840	H	-4.9714	0.8701	0.9936
C	1.1011	-0.3960	0.2727	C	-4.1847	-1.4651	-0.0571	H	-5.2278	-1.4320	0.2777
C	0.2783	0.7662	0.0029	C	-3.6918	-2.5751	-0.6997	H	-4.3293	-3.4485	-0.8710
C	2.4530	-0.2639	-0.0026	C	-2.3660	-2.5809	-1.1662	H	-1.9973	-3.4448	-1.7291
C	3.4339	-1.2737	0.2072	H	5.6587	-1.2353	-0.1925	H	-0.3005	-1.7734	1.2132
C	3.0396	-2.4665	0.7570	H	5.2720	1.3073	-0.9508				

Table 3.188: Table of thermodynamic data as a function of temperature for Naphth[2,1-*l*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.763	504.227	504.227	∞
100	97.214	332.025	718.857	-38.683	527.604	567.195	-296.266
200	193.329	427.178	549.214	-24.407	515.197	611.732	-159.765
250	249.613	476.318	529.694	-13.344	509.385	636.539	-132.995
298.15	304.512	524.989	524.989	0.000	504.227	661.510	-115.891
300	306.595	526.879	524.995	0.565	504.037	662.485	-115.346
350	361.311	578.293	528.930	17.277	499.302	689.278	-102.867
400	411.953	629.897	538.327	36.628	495.206	716.696	-93.589
450	457.740	681.111	551.353	58.391	491.670	744.599	-86.429
500	498.597	731.495	566.856	82.319	488.612	772.888	-80.741
600	566.976	828.694	602.469	135.735	483.653	830.235	-72.277
700	620.963	920.307	641.399	195.236	480.035	888.308	-66.285
800	664.231	1006.152	681.688	259.572	477.596	946.803	-61.819
900	699.490	1086.491	722.252	327.816	476.182	1005.535	-58.359
1000	728.626	1161.745	762.479	399.266	475.653	1064.388	-55.597
1100	752.968	1232.366	802.019	473.382	475.839	1123.266	-53.338
1200	773.482	1298.787	840.677	549.733	476.620	1182.084	-51.454
1300	790.895	1361.405	878.348	627.975	477.840	1240.829	-49.856
1400	805.769	1420.575	914.984	707.827	479.384	1299.470	-48.483
1500	818.546	1476.614	950.575	789.059	481.184	1357.993	-47.289
1600	829.581	1529.803	985.129	871.478	483.126	1416.382	-46.239
1700	839.160	1580.390	1018.668	954.927	485.148	1474.627	-45.309
1800	847.514	1628.597	1051.225	1039.270	487.185	1532.807	-44.480
1900	854.834	1674.620	1082.833	1124.395	489.211	1590.829	-43.734
2000	861.275	1718.634	1113.531	1210.207	491.177	1648.768	-43.061
2100	866.968	1760.797	1143.356	1296.625	493.017	1706.599	-42.448
2200	872.018	1801.247	1172.347	1383.579	494.730	1764.348	-41.890
2300	876.516	1840.111	1200.541	1471.010	496.312	1822.021	-41.379
2400	880.537	1877.502	1227.974	1558.867	497.701	1879.586	-40.907
2500	884.144	1913.521	1254.680	1647.104	498.909	1937.198	-40.475
2600	887.389	1948.262	1280.692	1735.683	499.902	1994.662	-40.072
2700	890.319	1981.809	1306.041	1824.571	500.686	2052.156	-39.701
2800	892.972	2014.236	1330.758	1913.738	501.238	2109.644	-39.355
2900	895.381	2045.614	1354.870	2003.157	501.531	2167.070	-39.032
3000	897.574	2076.007	1378.404	2092.807	501.606	2224.512	-38.731
3100	899.576	2105.471	1401.385	2182.666	501.393	2281.890	-38.449
3200	901.408	2134.061	1423.837	2272.716	500.929	2339.342	-38.185
3300	903.088	2161.825	1445.782	2362.942	500.199	2396.849	-37.938
3400	904.632	2188.808	1467.240	2453.329	499.178	2454.305	-37.705
3500	906.055	2215.052	1488.233	2543.865	497.870	2511.779	-37.485
3600	907.368	2240.595	1508.779	2634.537	496.295	2569.371	-37.280
3700	908.583	2265.472	1528.895	2725.335	494.426	2627.026	-37.086
3800	909.708	2289.718	1548.599	2816.250	492.238	2684.683	-36.903
3900	910.753	2313.362	1567.907	2907.274	489.769	2742.355	-36.729
4000	911.724	2336.432	1586.833	2998.398	487.003	2800.218	-36.566
4100	912.629	2358.956	1605.391	3089.617	483.910	2858.087	-36.412
4200	913.473	2380.959	1623.596	3180.922	480.515	2916.029	-36.265
4300	914.261	2402.463	1641.460	3272.309	476.804	2973.975	-36.126
4400	914.998	2423.490	1658.996	3363.773	472.786	3032.092	-35.995
4500	915.689	2444.060	1676.214	3455.307	468.474	3090.354	-35.871
4600	916.337	2464.193	1693.126	3546.909	463.822	3148.722	-35.754
4700	916.946	2483.907	1709.742	3638.574	458.842	3207.094	-35.642
4800	917.519	2503.217	1726.072	3730.297	453.577	3265.669	-35.537
4900	918.058	2522.142	1742.126	3822.076	447.960	3324.237	-35.436
5000	918.566	2540.694	1757.912	3913.908	442.074	3383.089	-35.342

3.189. Naphth[2,1-*e*]aceanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-35-9
Point Group: C₁

Length: 14.16 Å
Width: 10.57 Å
Breadth: 4.633 Å
L/B Ratio: 1.340

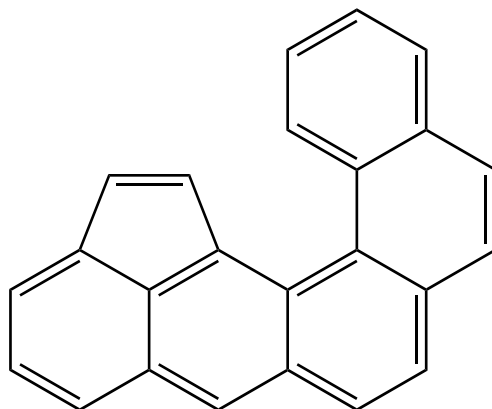
Cartesian coordinates:

C	2.0920	1.9528	-0.4581	C	-0.1327	-0.0937	0.0069	H	-4.6481	3.6107	0.3807
C	2.3311	0.6067	-0.0771	C	-0.7841	1.1310	0.1708	H	-6.0853	1.6195	0.0695
C	3.6723	0.2381	0.1678	C	-2.1901	1.2314	0.1445	H	-5.0667	-0.6410	-0.1850
C	4.7006	1.2140	0.1571	C	-3.0268	0.0899	-0.0234	H	-2.1794	3.3920	0.4329
C	4.4187	2.5184	-0.1534	C	-2.3915	-1.1511	-0.1336	H	-0.2102	2.0531	0.3418
C	3.1008	2.8816	-0.4912	C	-4.4441	0.2507	-0.0498	H	1.1419	-3.8717	0.0350
C	4.0123	-1.1290	0.3850	C	-4.9986	1.4874	0.0900	H	3.3166	-3.1464	0.4092
C	3.0536	-2.0872	0.3008	C	-4.1726	2.6309	0.2671	H	5.0573	-1.3900	0.5880
C	1.6839	-1.7406	0.0962	C	-2.8159	2.5101	0.2951	H	5.7258	0.9055	0.3926
C	1.2945	-0.3938	0.0072	C	-2.8632	-2.5398	-0.2376	H	5.2080	3.2769	-0.1603
C	0.7560	-2.8466	0.0007	C	-1.7902	-3.3787	-0.2378	H	2.8902	3.9139	-0.7901
C	-0.5607	-2.5786	-0.1343	H	-3.9150	-2.8128	-0.3011	H	1.0832	2.2609	-0.7626
C	-0.9892	-1.1993	-0.1055	H	-1.7976	-4.4647	-0.2994				

Table 3.189: Table of thermodynamic data as a function of temperature for Naphth[2,1-*e*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.961	489.589	489.589	∞
100	98.510	334.661	722.710	-38.805	512.844	552.172	-288.419
200	193.937	430.582	552.693	-24.422	500.545	596.399	-155.760
250	249.740	479.803	533.169	-13.341	494.750	621.033	-129.755
298.15	304.290	528.466	528.466	0.000	489.589	645.836	-113.145
300	306.362	530.354	528.471	0.565	489.399	646.804	-112.616
350	360.837	581.713	532.403	17.258	484.645	673.425	-100.501
400	411.333	633.243	541.789	36.582	480.522	700.674	-91.497
450	457.041	684.379	554.797	58.312	476.952	728.411	-84.550
500	497.866	734.688	570.279	82.204	473.859	756.539	-79.033
600	566.256	831.753	605.842	135.547	468.827	813.573	-70.826
700	620.299	923.259	644.720	194.978	465.140	871.346	-65.019
800	663.632	1009.020	684.956	259.251	462.638	929.550	-60.692
900	698.954	1089.292	725.472	327.438	461.167	987.999	-57.341
1000	728.148	1164.492	765.654	398.838	460.587	1046.575	-54.666
1100	752.540	1235.070	805.154	472.908	460.728	1105.180	-52.480
1200	773.099	1301.456	843.774	549.219	461.468	1163.730	-50.655
1300	790.550	1364.045	881.411	627.424	462.651	1222.209	-49.108
1400	805.457	1423.191	918.016	707.244	464.163	1280.587	-47.778
1500	818.264	1479.209	953.578	788.446	465.933	1338.850	-46.622
1600	829.325	1532.380	988.106	870.839	467.848	1396.981	-45.606
1700	838.926	1582.953	1021.622	954.262	469.846	1454.968	-44.705
1800	847.300	1631.147	1054.156	1038.583	471.861	1512.893	-43.902
1900	854.638	1677.159	1085.744	1123.688	473.866	1570.660	-43.180
2000	861.095	1721.163	1116.423	1209.481	475.813	1628.346	-42.527
2100	866.801	1763.317	1146.231	1295.882	477.636	1685.924	-41.934
2200	871.864	1803.760	1175.206	1382.820	479.333	1743.422	-41.393
2300	876.374	1842.617	1203.384	1470.236	480.900	1800.844	-40.898
2400	880.405	1880.002	1230.803	1558.079	482.276	1858.159	-40.441
2500	884.020	1916.017	1257.495	1646.303	483.470	1915.521	-40.022
2600	887.274	1950.753	1283.495	1734.871	484.452	1972.735	-39.632
2700	890.212	1984.295	1308.833	1823.748	485.224	2029.980	-39.272
2800	892.871	2016.719	1333.539	1912.904	485.766	2087.220	-38.937
2900	895.286	2048.094	1357.641	2002.314	486.050	2144.398	-38.624
3000	897.485	2078.483	1381.165	2091.954	486.115	2201.593	-38.332
3100	899.492	2107.945	1404.137	2181.804	485.893	2258.722	-38.058
3200	901.329	2136.532	1426.580	2271.847	485.421	2315.928	-37.803
3300	903.013	2164.293	1448.516	2362.065	484.684	2373.187	-37.564
3400	904.562	2191.274	1469.967	2452.445	483.656	2430.396	-37.338
3500	905.988	2217.516	1490.952	2542.973	482.341	2487.624	-37.125
3600	907.305	2243.057	1511.491	2633.639	480.760	2544.970	-36.926
3700	908.522	2267.933	1531.601	2724.431	478.884	2602.379	-36.738
3800	909.651	2292.177	1551.298	2815.340	476.690	2659.789	-36.561
3900	910.698	2315.819	1570.599	2906.358	474.215	2717.216	-36.392
4000	911.672	2338.889	1589.519	2997.477	471.444	2774.833	-36.235
4100	912.579	2361.412	1608.073	3088.690	468.346	2832.457	-36.085
4200	913.425	2383.413	1626.272	3179.991	464.946	2890.153	-35.944
4300	914.216	2404.916	1644.131	3271.374	461.230	2947.854	-35.809
4400	914.955	2425.941	1661.661	3362.833	457.208	3005.726	-35.682
4500	915.648	2446.511	1678.875	3454.363	452.892	3063.743	-35.562
4600	916.297	2466.643	1695.782	3545.961	448.236	3121.865	-35.449
4700	916.908	2486.356	1712.394	3637.621	443.252	3179.993	-35.341
4800	917.482	2505.666	1728.720	3729.341	437.983	3238.323	-35.239
4900	918.022	2524.589	1744.770	3821.116	432.362	3296.646	-35.142
5000	918.532	2543.141	1760.552	3912.944	426.473	3355.253	-35.051

3.190. Naphth[2,1-*l*]aceanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-43-9
Point Group: C₁

Length: 13.93 Å
Width: 10.14 Å
Breadth: 5.678 Å
L/B Ratio: 1.374

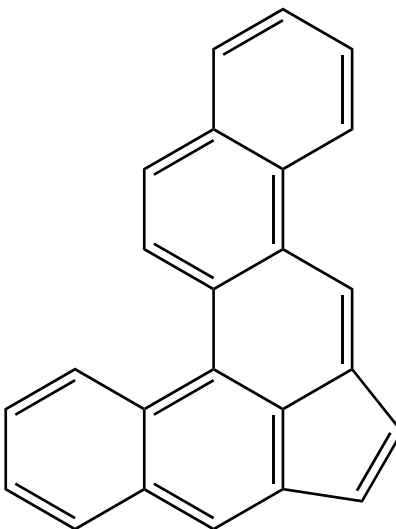
Cartesian coordinates:

C	1.6607	-1.5997	0.8344	C	-3.0271	-1.5475	-0.4502	H	-4.9311	-2.5455	-0.5745
C	-0.7620	-1.7719	-0.8341	C	1.8839	1.9509	-0.2545	H	-6.1773	-0.5792	0.2750
C	-0.9773	-0.4220	-0.2758	C	1.1491	3.1750	-0.0876	H	-5.0494	1.5509	0.8331
C	-0.1872	0.6857	0.0167	C	-0.1526	3.1508	0.2728	H	-2.7452	2.9184	0.7778
C	1.2644	0.7213	-0.0309	C	3.4729	-0.3505	-0.1795	H	-0.6928	4.0788	0.4939
C	2.1098	-0.4264	0.1772	C	4.0240	0.8872	-0.6282	H	1.6864	4.1227	-0.2085
C	-0.8873	1.9104	0.3062	C	3.2659	2.0160	-0.6015	H	3.6969	2.9900	-0.8603
C	-2.2664	1.9674	0.5152	C	2.4955	-2.6742	1.0131	H	5.0731	0.9164	-0.9436
C	-3.0558	0.8177	0.3407	C	3.8247	-2.6308	0.5483	H	5.3524	-1.4218	-0.3569
C	-2.3784	-0.3194	-0.0899	C	4.3095	-1.4836	-0.0256	H	4.4671	-3.5088	0.6701
C	-4.4732	0.6896	0.4788	C	-1.9515	-2.4290	-0.9266	H	2.1361	-3.5724	1.5260
C	-5.0907	-0.4921	0.1644	H	-2.1205	-3.4361	-1.3016	H	0.2149	-2.1452	-1.1418
C	-4.3809	-1.6349	-0.3187	H	0.6362	-1.6297	1.2291				

Table 3.190: Table of thermodynamic data as a function of temperature for Naphth[2,1-*l*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-44.755	512.166	512.166	∞
100	96.946	332.127	719.039	-38.691	535.535	575.116	-300.403
200	193.405	427.198	549.323	-24.425	523.119	619.650	-161.833
250	249.809	476.369	529.788	-13.355	517.313	644.455	-134.649
298.15	304.755	525.079	525.079	0.000	512.166	669.422	-117.278
300	306.838	526.971	525.085	0.566	511.977	670.397	-116.724
350	361.556	578.423	529.024	17.290	507.254	697.185	-104.047
400	412.181	630.058	538.427	36.653	503.170	724.596	-94.621
450	457.944	681.297	551.461	58.426	499.644	752.490	-87.345
500	498.777	731.702	566.973	82.365	496.596	780.769	-81.565
600	567.120	828.931	602.603	135.797	491.653	838.093	-72.961
700	621.083	920.564	641.550	195.310	488.049	896.142	-66.870
800	664.335	1006.424	681.853	259.657	485.621	954.610	-62.328
900	699.583	1086.775	722.429	327.911	484.217	1013.315	-58.810
1000	728.710	1162.038	762.667	399.370	483.696	1072.139	-56.002
1100	753.045	1232.666	802.218	473.494	483.891	1130.987	-53.705
1200	773.553	1299.094	840.884	549.852	484.679	1189.775	-51.788
1300	790.960	1361.717	878.563	628.101	485.905	1248.489	-50.164
1400	805.828	1420.892	915.207	707.960	487.456	1307.098	-48.767
1500	818.601	1476.935	950.804	789.197	489.261	1365.590	-47.553
1600	829.632	1530.127	985.363	871.622	491.209	1423.947	-46.486
1700	839.207	1580.717	1018.908	955.075	493.236	1482.158	-45.540
1800	847.558	1628.926	1051.470	1039.422	495.277	1540.306	-44.698
1900	854.874	1674.952	1083.082	1124.552	497.307	1598.295	-43.939
2000	861.313	1718.968	1113.784	1210.368	499.277	1656.200	-43.255
2100	867.003	1761.132	1143.614	1296.790	501.121	1713.998	-42.632
2200	872.051	1801.584	1172.608	1383.747	502.837	1771.713	-42.065
2300	876.547	1840.449	1200.805	1471.181	504.422	1829.352	-41.545
2400	880.566	1877.841	1228.241	1559.041	505.815	1886.884	-41.066
2500	884.170	1913.862	1254.950	1647.281	507.025	1944.461	-40.626
2600	887.414	1948.604	1280.965	1735.863	508.021	2001.891	-40.218
2700	890.343	1982.152	1306.317	1824.753	508.807	2059.351	-39.840
2800	892.994	2014.580	1331.036	1913.922	509.361	2116.805	-39.489
2900	895.402	2045.959	1355.151	2003.344	509.657	2174.196	-39.161
3000	897.593	2076.352	1378.687	2092.995	509.733	2231.604	-38.855
3100	899.594	2105.817	1401.670	2182.856	509.522	2288.947	-38.568
3200	901.425	2134.407	1424.123	2272.908	509.060	2346.365	-38.300
3300	903.104	2162.172	1446.070	2363.136	508.332	2403.837	-38.049
3400	904.648	2189.155	1467.530	2453.525	507.313	2461.258	-37.812
3500	906.070	2215.400	1488.525	2544.062	506.006	2518.697	-37.589
3600	907.382	2240.943	1509.072	2634.735	504.433	2576.255	-37.380
3700	908.596	2265.821	1529.190	2725.535	502.565	2633.875	-37.183
3800	909.721	2290.067	1548.895	2816.451	500.378	2691.497	-36.996
3900	910.765	2313.711	1568.204	2907.476	497.910	2749.134	-36.820
4000	911.736	2336.782	1587.131	2998.602	495.146	2806.962	-36.654
4100	912.640	2359.306	1605.691	3089.821	492.054	2864.797	-36.497
4200	913.483	2381.309	1623.898	3181.128	488.660	2922.703	-36.348
4300	914.271	2402.813	1641.763	3272.516	484.950	2980.614	-36.207
4400	915.008	2423.840	1659.299	3363.980	480.933	3038.696	-36.073
4500	915.699	2444.411	1676.518	3455.516	476.622	3096.923	-35.947
4600	916.346	2464.544	1693.431	3547.119	471.971	3155.256	-35.828
4700	916.955	2484.258	1710.048	3638.784	466.992	3213.593	-35.714
4800	917.527	2503.569	1726.380	3730.508	461.727	3272.133	-35.607
4900	918.066	2522.493	1742.434	3822.288	456.111	3330.666	-35.505
5000	918.573	2541.046	1758.222	3914.120	450.226	3389.482	-35.409

3.191. Benzo[*c*]cyclopenta[*qr*]chrysene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-51-9
Point Group: C₁

Length: 14.60 Å
Width: 10.51 Å
Breadth: 4.541 Å
L/B Ratio: 1.389

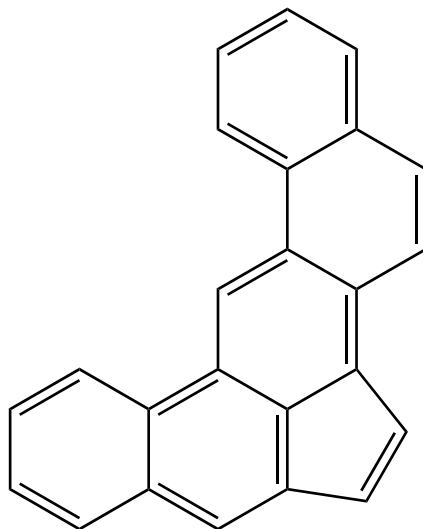
Cartesian coordinates:

C	-1.1514	1.3164	-0.0268	C	1.1729	1.9131	0.0933	H	-3.2994	-4.0386	0.5432
C	-2.4296	1.9787	-0.0920	C	0.4409	-0.4529	-0.1000	H	-5.4853	-2.9236	0.1394
C	-2.1469	3.4227	-0.0794	C	1.4632	0.5138	0.0210	H	-5.5691	-0.4650	-0.1902
C	-0.8038	3.6167	-0.0010	C	2.1250	-2.1964	-0.3926	H	-1.2166	-2.7529	0.5159
C	-0.1253	2.3115	0.0261	C	0.8259	-1.8055	-0.3674	H	-4.5509	1.6747	-0.2493
C	-3.3289	-2.9620	0.3449	C	3.1730	-1.2562	-0.1530	H	1.9978	2.6351	0.1796
C	-4.5641	-2.3323	0.1336	C	2.8480	0.0979	0.0383	H	2.3943	-3.2379	-0.6038
C	-4.6058	-0.9718	-0.0569	C	3.9036	1.0187	0.2482	H	0.0474	-2.5460	-0.5935
C	-2.1617	-2.2337	0.3100	C	5.2112	0.5997	0.2731	H	3.6592	2.0817	0.3930
C	-2.1590	-0.8456	0.0506	C	5.5269	-0.7589	0.0854	H	6.0186	1.3203	0.4397
C	-3.4195	-0.2032	-0.0713	C	4.5245	-1.6731	-0.1264	H	6.5742	-1.0769	0.1092
C	-3.5542	1.2296	-0.1588	H	-2.9239	4.1832	-0.1244	H	4.7574	-2.7334	-0.2761
C	-0.9437	-0.0489	-0.0257	H	-0.2733	4.5661	0.0342				

Table 3.191: Table of thermodynamic data as a function of temperature for Benzo[*c*]cyclopenta[*qr*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.067	474.509	474.509	∞
100	98.875	336.776	725.189	-38.841	497.728	536.844	-280.413
200	194.109	432.898	555.052	-24.431	485.456	580.847	-151.699
250	249.818	482.147	535.522	-13.344	479.667	605.365	-126.481
298.15	304.316	530.818	530.818	0.000	474.509	630.055	-110.381
300	306.386	532.707	530.824	0.565	474.319	631.018	-109.868
350	360.829	584.067	534.756	17.259	469.566	657.522	-98.128
400	411.301	635.594	544.141	36.581	465.441	684.653	-89.405
450	456.988	686.725	557.149	58.309	461.870	712.273	-82.677
500	497.793	737.027	572.630	82.198	458.773	740.283	-77.335
600	566.151	834.076	608.190	135.532	453.732	797.085	-69.391
700	620.166	925.564	647.063	194.951	450.033	854.626	-63.772
800	663.480	1011.305	687.293	259.210	447.517	912.600	-59.585
900	698.790	1091.559	727.802	327.381	446.030	970.822	-56.344
1000	727.977	1166.742	767.977	398.764	445.433	1029.172	-53.757
1100	752.368	1237.303	807.469	472.817	445.557	1087.553	-51.643
1200	772.928	1303.674	846.082	549.110	446.280	1145.881	-49.878
1300	790.384	1366.249	883.711	627.299	447.446	1204.139	-48.382
1400	805.298	1425.383	920.310	707.102	448.942	1262.297	-47.096
1500	818.112	1481.391	955.865	788.289	450.696	1320.341	-45.977
1600	829.181	1534.552	990.385	870.667	452.597	1378.254	-44.994
1700	838.790	1585.116	1023.895	954.076	454.581	1436.025	-44.123
1800	847.172	1633.303	1056.423	1038.384	456.582	1493.734	-43.346
1900	854.517	1679.308	1088.005	1123.476	458.574	1551.286	-42.647
2000	860.981	1723.307	1118.678	1209.258	460.510	1608.757	-42.016
2100	866.694	1765.455	1148.480	1295.647	462.322	1666.121	-41.442
2200	871.764	1805.893	1177.450	1382.575	464.008	1723.405	-40.918
2300	876.279	1844.746	1205.624	1469.982	465.566	1780.614	-40.438
2400	880.316	1882.127	1233.037	1557.815	466.932	1837.716	-39.996
2500	883.937	1918.138	1259.726	1646.031	468.118	1894.866	-39.590
2600	887.195	1952.871	1285.721	1734.590	469.092	1951.869	-39.213
2700	890.137	1986.410	1311.055	1823.460	469.857	2008.902	-38.864
2800	892.801	2018.831	1335.757	1912.609	470.391	2065.930	-38.540
2900	895.220	2050.204	1359.855	2002.012	470.668	2122.897	-38.237
3000	897.422	2080.591	1383.376	2091.645	470.726	2179.881	-37.954
3100	899.432	2110.050	1406.344	2181.489	470.499	2236.800	-37.689
3200	901.272	2138.636	1428.784	2271.526	470.021	2293.795	-37.442
3300	902.959	2166.396	1450.717	2361.739	469.278	2350.844	-37.210
3400	904.510	2193.375	1472.165	2452.113	468.245	2407.843	-36.991
3500	905.939	2219.615	1493.148	2542.637	466.925	2464.860	-36.785
3600	907.258	2245.155	1513.684	2633.298	465.339	2521.996	-36.592
3700	908.478	2270.030	1533.791	2724.085	463.458	2579.196	-36.411
3800	909.609	2294.273	1553.486	2814.990	461.260	2636.397	-36.239
3900	910.658	2317.914	1572.785	2906.004	458.781	2693.614	-36.076
4000	911.634	2340.982	1591.702	2997.119	456.007	2751.021	-35.924
4100	912.542	2363.504	1610.253	3088.329	452.905	2808.436	-35.779
4200	913.390	2385.505	1628.451	3179.626	449.501	2865.923	-35.642
4300	914.182	2407.006	1646.308	3271.005	445.782	2923.414	-35.512
4400	914.923	2428.032	1663.836	3362.460	441.757	2981.078	-35.389
4500	915.617	2448.600	1681.048	3453.988	437.437	3038.885	-35.274
4600	916.268	2468.732	1697.953	3545.582	432.778	3096.799	-35.165
4700	916.879	2488.444	1714.563	3637.240	427.791	3154.718	-35.060
4800	917.454	2507.753	1730.887	3728.957	422.519	3212.839	-34.962
4900	917.996	2526.676	1746.936	3820.730	416.896	3270.953	-34.868
5000	918.506	2545.227	1762.716	3912.555	411.004	3329.352	-34.781

3.192. Dibenz[*e,j*]aceanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 53974-16-6
Point Group: C_s

Length: 14.44 Å
Width: 10.58 Å
Breadth: 3.885 Å
L/B Ratio: 1.366

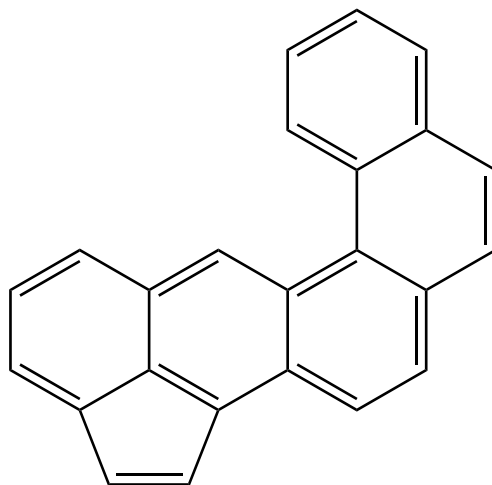
Cartesian coordinates:

C	1.1210	1.1689	0.0000	C	-1.2778	1.3648	0.0000	H	-4.0604	-3.8105	0.0000
C	2.3104	1.9916	0.0000	C	-1.3203	-0.0619	0.0000	H	-1.8222	-2.7231	0.0000
C	1.8173	3.3791	0.0000	C	-0.1470	-0.8311	0.0000	H	-5.9585	0.0535	0.0000
C	0.4548	3.3717	0.0000	C	1.1118	-0.2212	0.0000	H	-6.1233	-2.4264	0.0000
C	-0.0275	1.9807	0.0000	C	3.5211	1.3903	0.0000	H	-2.4219	3.2162	0.0000
C	-3.9793	-2.7186	0.0000	C	3.5799	-0.0595	0.0000	H	-4.6334	2.0810	0.0000
C	-2.7401	-2.1157	0.0000	C	2.4135	-0.8608	0.0000	H	-0.2187	-1.9323	0.0000
C	-5.0519	-0.5624	0.0000	C	2.5336	-2.2615	0.0000	H	4.4577	1.9585	0.0000
C	-5.1437	-1.9375	0.0000	C	3.7776	-2.8578	0.0000	H	1.6182	-2.8684	0.0000
C	-3.7913	0.0679	0.0000	C	4.9352	-2.0688	0.0000	H	3.8658	-3.9492	0.0000
C	-2.6208	-0.7111	0.0000	C	4.8387	-0.6926	0.0000	H	5.9181	-2.5514	0.0000
C	-2.4995	2.1227	0.0000	H	2.4722	4.2479	0.0000	H	5.7469	-0.0785	0.0000
C	-3.7010	1.5047	0.0000	H	-0.2077	4.2355	0.0000				

Table 3.192: Table of thermodynamic data as a function of temperature for Dibenz[*e,j*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-45.188	457.650	457.650	∞
100	99.735	338.554	727.493	-38.894	480.816	519.754	-271.486
200	194.326	435.058	557.218	-24.432	468.596	563.555	-147.182
250	249.822	484.332	537.690	-13.339	462.812	587.963	-122.846
298.15	304.145	532.989	532.989	0.000	457.650	612.548	-107.314
300	306.209	534.876	532.994	0.565	457.459	613.508	-106.819
350	360.509	586.198	536.924	17.246	452.694	639.904	-95.498
400	410.881	637.675	546.302	36.549	448.550	666.930	-87.090
450	456.511	688.752	559.298	58.255	444.956	694.447	-80.608
500	497.293	739.003	574.764	82.120	441.835	722.357	-75.463
600	565.673	835.962	610.289	135.404	436.745	778.966	-67.814
700	619.756	927.381	649.127	194.778	433.001	836.322	-62.406
800	663.151	1013.073	689.323	259.000	430.448	894.117	-58.379
900	698.536	1093.292	729.801	327.142	428.932	952.164	-55.261
1000	727.787	1168.451	769.948	398.503	428.313	1010.341	-52.774
1100	752.230	1238.997	809.416	472.540	428.420	1068.553	-50.740
1200	772.831	1305.358	848.007	548.821	429.132	1126.711	-49.043
1300	790.318	1367.927	885.617	627.002	430.290	1184.801	-47.605
1400	805.255	1427.056	922.199	706.800	431.780	1242.792	-46.368
1500	818.087	1483.062	957.740	787.983	433.531	1300.669	-45.292
1600	829.170	1536.222	992.248	870.359	435.430	1358.415	-44.347
1700	838.789	1586.786	1025.746	953.768	437.413	1416.018	-43.508
1800	847.178	1634.973	1058.264	1038.076	439.415	1473.561	-42.761
1900	854.528	1680.978	1089.837	1123.169	441.408	1530.945	-42.088
2000	860.996	1724.978	1120.502	1208.952	443.345	1588.249	-41.480
2100	866.712	1767.127	1150.297	1295.344	445.158	1645.447	-40.927
2200	871.784	1807.566	1179.260	1382.273	446.847	1702.563	-40.423
2300	876.300	1846.420	1207.428	1469.682	448.407	1759.605	-39.961
2400	880.337	1883.802	1234.836	1557.517	449.775	1816.540	-39.535
2500	883.959	1919.814	1261.519	1645.735	450.963	1873.522	-39.144
2600	887.217	1954.548	1287.510	1734.297	451.939	1930.357	-38.781
2700	890.159	1988.088	1312.840	1823.168	452.706	1987.222	-38.444
2800	892.822	2020.510	1337.538	1912.320	453.242	2044.083	-38.132
2900	895.241	2051.883	1361.633	2001.725	453.521	2100.882	-37.840
3000	897.443	2082.270	1385.150	2091.360	453.582	2157.698	-37.568
3100	899.452	2111.731	1408.116	2181.207	453.356	2214.449	-37.312
3200	901.292	2140.317	1430.552	2271.245	452.881	2271.276	-37.074
3300	902.978	2168.077	1452.483	2361.460	452.140	2328.157	-36.851
3400	904.529	2195.057	1473.929	2451.836	451.108	2384.988	-36.640
3500	905.957	2221.298	1494.909	2542.362	449.790	2441.837	-36.442
3600	907.276	2246.838	1515.443	2633.024	448.206	2498.805	-36.256
3700	908.495	2271.713	1535.548	2723.814	446.327	2555.836	-36.081
3800	909.625	2295.957	1555.241	2814.720	444.131	2612.868	-35.916
3900	910.674	2319.598	1574.538	2905.736	441.654	2669.917	-35.759
4000	911.649	2342.667	1593.454	2996.853	438.880	2727.156	-35.612
4100	912.557	2365.189	1612.003	3088.063	435.780	2784.402	-35.473
4200	913.404	2387.190	1630.199	3179.362	432.378	2841.720	-35.341
4300	914.195	2408.692	1648.054	3270.742	428.660	2899.044	-35.216
4400	914.936	2429.718	1665.582	3362.199	424.636	2956.538	-35.098
4500	915.629	2450.287	1682.792	3453.728	420.318	3014.177	-34.987
4600	916.280	2470.419	1699.696	3545.324	415.659	3071.923	-34.882
4700	916.891	2490.131	1716.305	3636.983	410.674	3129.672	-34.782
4800	917.466	2509.441	1732.628	3728.701	405.403	3187.625	-34.688
4900	918.007	2528.364	1748.675	3820.475	399.781	3245.571	-34.597
5000	918.517	2546.915	1764.455	3912.301	393.891	3303.800	-34.514

3.193. Naphth[1,2-*j*]aceanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-59-7
Point Group: C₁

Length: 14.06 Å
Width: 10.08 Å
Breadth: 4.953 Å
L/B Ratio: 1.395

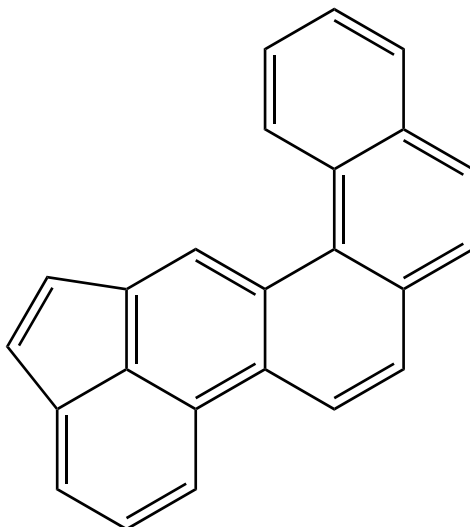
Cartesian coordinates:

C	2.1494	1.7980	0.5791	C	-0.0243	-0.2983	-0.0308	H	-4.5370	3.4086	-0.6087
C	2.4209	0.4898	0.1010	C	-2.2684	-1.2102	0.2205	H	-5.9058	1.4010	-0.1323
C	3.7690	0.1789	-0.1840	C	-2.7503	0.0990	0.0123	H	-2.0693	3.3304	-0.7204
C	4.7681	1.1820	-0.1180	C	-1.9481	1.1992	-0.2669	H	0.0973	1.8147	-0.5262
C	4.4546	2.4515	0.2924	C	-0.5611	0.9671	-0.2901	H	-1.0560	-3.5877	0.3840
C	3.1323	2.7506	0.6714	C	-2.6464	2.4269	-0.4966	H	1.3640	-3.9820	-0.0507
C	4.1496	-1.1617	-0.4884	C	-4.0148	2.4612	-0.4344	H	3.5176	-3.2015	-0.5824
C	3.2281	-2.1567	-0.4195	C	-4.8158	1.3087	-0.1556	H	5.1955	-1.3736	-0.7378
C	1.8575	-1.8592	-0.1577	C	-4.1836	0.1219	0.0662	H	5.7981	0.9216	-0.3878
C	1.4153	-0.5410	-0.0277	C	-4.5804	-1.2690	0.3414	H	5.2225	3.2298	0.3460
C	0.9528	-2.9664	-0.0108	C	-3.4634	-2.0469	0.4241	H	2.8962	3.7518	1.0473
C	-0.3627	-2.7568	0.2095	H	-5.6146	-1.5879	0.4522	H	1.1307	2.0551	0.9000
C	-0.8980	-1.4261	0.1629	H	-3.4219	-3.1177	0.6150				

Table 3.193: Table of thermodynamic data as a function of temperature for Naphth[1,2-*j*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.878	502.634	502.634	∞
100	97.741	334.635	722.011	-38.738	525.957	565.287	-295.270
200	193.589	430.074	552.184	-24.422	513.590	609.546	-159.194
250	249.763	479.259	532.654	-13.349	507.788	634.207	-132.508
298.15	304.556	527.948	527.948	0.000	502.634	659.036	-115.458
300	306.634	529.838	527.954	0.565	502.445	660.005	-114.915
350	361.249	581.251	531.890	17.276	497.709	686.650	-102.475
400	411.811	632.841	541.285	36.622	493.608	713.921	-93.227
450	457.539	684.034	554.308	58.377	490.063	741.677	-86.090
500	498.358	734.395	569.807	82.294	486.995	769.820	-80.421
600	566.704	831.547	605.407	135.684	482.009	826.880	-71.985
700	620.689	923.118	644.323	195.157	478.364	884.669	-66.013
800	663.970	1008.927	684.595	259.466	475.899	942.885	-61.563
900	699.246	1089.236	725.142	327.685	474.459	1001.341	-58.115
1000	728.401	1164.465	765.354	399.112	473.906	1059.921	-55.363
1100	752.761	1235.066	804.879	473.206	474.071	1118.528	-53.113
1200	773.292	1301.470	843.522	549.537	474.832	1177.077	-51.236
1300	790.721	1364.073	881.180	627.761	476.033	1235.554	-49.644
1400	805.609	1423.231	917.805	707.596	477.561	1293.929	-48.276
1500	818.400	1479.259	953.384	788.813	479.345	1352.187	-47.086
1600	829.447	1532.439	987.927	871.218	481.274	1410.313	-46.041
1700	839.036	1583.018	1021.457	954.653	483.283	1468.294	-45.114
1800	847.400	1631.218	1054.004	1038.985	485.308	1526.212	-44.289
1900	854.728	1677.235	1085.604	1124.099	487.322	1583.972	-43.546
2000	861.178	1721.244	1116.294	1209.901	489.278	1641.649	-42.875
2100	866.877	1763.402	1146.112	1296.310	491.109	1699.220	-42.265
2200	871.934	1803.848	1175.096	1383.255	492.814	1756.708	-41.709
2300	876.439	1842.709	1203.283	1470.678	494.388	1814.121	-41.199
2400	880.465	1880.096	1230.710	1558.527	495.769	1871.427	-40.730
2500	884.076	1916.113	1257.410	1646.757	496.970	1928.779	-40.299
2600	887.326	1950.852	1283.417	1735.330	497.957	1985.984	-39.898
2700	890.260	1984.395	1308.761	1824.212	498.734	2043.219	-39.528
2800	892.916	2016.821	1333.474	1913.373	499.280	2100.449	-39.184
2900	895.328	2048.197	1357.581	2002.787	499.568	2157.616	-38.862
3000	897.524	2078.588	1381.111	2092.431	499.638	2214.801	-38.562
3100	899.529	2108.051	1404.088	2182.285	499.420	2271.920	-38.281
3200	901.364	2136.639	1426.535	2272.331	498.952	2329.115	-38.018
3300	903.046	2164.402	1448.476	2362.553	498.218	2386.363	-37.772
3400	904.593	2191.383	1469.932	2452.936	497.193	2443.562	-37.540
3500	906.017	2217.626	1490.921	2543.468	495.881	2500.778	-37.321
3600	907.333	2243.168	1511.464	2634.136	494.302	2558.113	-37.116
3700	908.549	2268.045	1531.577	2724.931	492.429	2615.511	-36.924
3800	909.676	2292.290	1551.278	2815.843	490.238	2672.910	-36.741
3900	910.722	2315.933	1570.583	2906.863	487.766	2730.326	-36.568
4000	911.695	2339.002	1589.506	2997.985	484.997	2787.931	-36.406
4100	912.601	2361.526	1608.062	3089.200	481.902	2845.544	-36.252
4200	913.446	2383.528	1626.265	3180.503	478.503	2903.228	-36.106
4300	914.235	2405.031	1644.127	3271.887	474.790	2960.918	-35.967
4400	914.974	2426.057	1661.660	3363.348	470.770	3018.778	-35.837
4500	915.666	2446.627	1678.876	3454.881	466.455	3076.783	-35.714
4600	916.315	2466.760	1695.786	3546.480	461.800	3134.895	-35.597
4700	916.924	2486.473	1712.400	3638.142	456.819	3193.010	-35.486
4800	917.498	2505.783	1728.728	3729.864	451.551	3251.329	-35.381
4900	918.038	2524.707	1744.780	3821.641	445.932	3309.640	-35.280
5000	918.546	2543.259	1760.565	3913.470	440.045	3368.236	-35.187

3.194. Benzo[*c*]cyclopenta[*hi*]chrysene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-67-7
Point Group: C₁

Length: 14.39 Å
Width: 10.00 Å
Breadth: 4.982 Å
L/B Ratio: 1.439

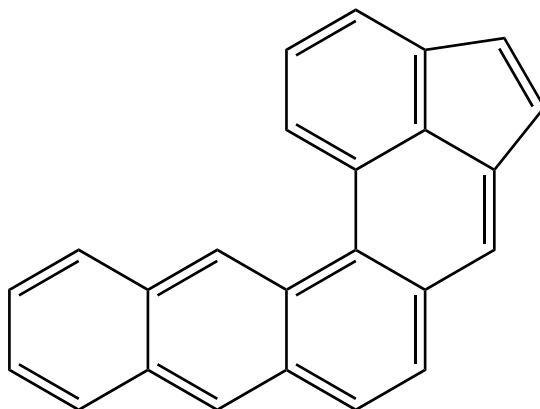
Cartesian coordinates:

C	-2.6925	-2.5739	0.5137	C	4.1184	1.2336	0.4571	H	0.2148	-1.9513	0.5543
C	-3.9974	-2.2101	0.3701	C	2.4620	-0.5100	-0.0903	H	-1.2244	3.3756	-0.3626
C	-4.0763	-0.7687	0.0726	C	3.7934	-0.1353	0.1900	H	1.2001	3.9153	-0.0222
C	-2.7304	-0.3130	0.0410	C	4.8337	-1.0912	0.1450	H	3.4063	3.2463	0.4863
C	-1.8293	-1.3969	0.3076	C	4.5774	-2.3832	-0.2449	H	5.1552	1.4920	0.7006
C	-0.4956	-1.1477	0.3201	C	3.2750	-2.7437	-0.6262	H	5.8512	-0.7828	0.4120
C	-0.0055	0.1850	0.0486	C	2.2497	-1.8302	-0.5533	H	5.3799	-3.1268	-0.2797
C	-0.9204	1.2470	-0.1225	C	-2.3402	0.9937	-0.1660	H	3.0818	-3.7589	-0.9885
C	-0.4714	2.5893	-0.2027	C	-5.0733	0.1506	-0.1370	H	1.2467	-2.1365	-0.8800
C	0.8492	2.8768	-0.0348	C	-4.7013	1.5002	-0.3648	H	-6.1302	-0.1320	-0.1265
C	1.4049	0.4803	0.0218	C	-3.3882	1.9245	-0.3765	H	-5.4991	2.2320	-0.5330
C	1.7963	1.8268	0.1076	H	-2.3071	-3.5658	0.7402	H	-3.1217	2.9778	-0.5426
C	3.1616	2.1855	0.3561	H	-4.8724	-2.8508	0.4589				

Table 3.194: Table of thermodynamic data as a function of temperature for Benzo[*c*]cyclopenta[*hi*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.853	484.636	484.636	∞
100	97.831	335.034	722.003	-38.697	508.000	547.290	-285.869
200	193.342	430.422	552.375	-24.391	495.624	591.510	-154.483
250	249.431	479.543	532.871	-13.332	489.807	616.155	-128.736
298.15	304.201	528.170	528.170	0.000	484.636	640.971	-112.293
300	306.279	530.058	528.176	0.565	484.446	641.940	-111.769
350	360.907	581.417	532.107	17.258	479.693	668.576	-99.777
400	411.496	632.963	541.494	36.588	475.575	695.839	-90.865
450	457.256	684.121	554.505	58.327	472.016	723.590	-83.990
500	498.103	734.454	569.992	82.231	468.934	751.730	-78.531
600	566.496	831.564	605.567	135.598	463.925	808.786	-70.410
700	620.515	923.105	644.460	195.052	460.261	866.575	-64.663
800	663.819	1008.892	684.711	259.345	457.779	924.793	-60.382
900	699.113	1089.185	725.241	327.549	456.326	983.254	-57.065
1000	728.283	1164.401	765.437	398.964	455.761	1041.840	-54.419
1100	752.655	1234.990	804.948	473.046	455.914	1100.454	-52.255
1200	773.196	1301.386	843.579	549.368	456.665	1159.011	-50.449
1300	790.634	1363.982	881.226	627.582	457.857	1217.497	-48.919
1400	805.530	1423.133	917.840	707.410	459.376	1275.881	-47.603
1500	818.327	1479.156	953.411	788.619	461.153	1334.149	-46.458
1600	829.381	1532.331	987.946	871.017	463.075	1392.285	-45.453
1700	838.975	1582.907	1021.468	954.446	465.078	1450.277	-44.561
1800	847.344	1631.104	1054.008	1038.772	467.097	1508.207	-43.766
1900	854.677	1677.118	1085.602	1123.881	469.106	1565.978	-43.051
2000	861.130	1721.125	1116.286	1209.678	471.057	1623.668	-42.405
2100	866.833	1763.280	1146.099	1296.082	472.883	1681.250	-41.818
2200	871.894	1803.724	1175.078	1383.023	474.583	1738.751	-41.282
2300	876.400	1842.583	1203.260	1470.442	476.153	1796.176	-40.792
2400	880.429	1879.969	1230.683	1558.287	477.532	1853.495	-40.339
2500	884.043	1915.984	1257.379	1646.514	478.728	1910.860	-39.924
2600	887.295	1950.722	1283.382	1735.084	479.712	1968.078	-39.538
2700	890.231	1984.264	1308.723	1823.962	480.487	2025.326	-39.181
2800	892.889	2016.689	1333.432	1913.120	481.030	2082.569	-38.850
2900	895.303	2048.064	1357.536	2002.532	481.315	2139.749	-38.540
3000	897.500	2078.454	1381.063	2092.174	481.382	2196.947	-38.251
3100	899.506	2107.916	1404.037	2182.026	481.162	2254.080	-37.980
3200	901.342	2136.504	1426.482	2272.069	480.692	2311.288	-37.727
3300	903.026	2164.266	1448.420	2362.289	479.955	2368.550	-37.490
3400	904.573	2191.247	1469.873	2452.670	478.929	2425.762	-37.267
3500	905.999	2217.489	1490.861	2543.200	477.615	2482.992	-37.056
3600	907.315	2243.031	1511.401	2633.866	476.035	2540.341	-36.859
3700	908.532	2267.907	1531.513	2724.659	474.160	2597.753	-36.673
3800	909.660	2292.151	1551.212	2815.570	471.967	2655.166	-36.497
3900	910.707	2315.794	1570.514	2906.589	469.493	2712.595	-36.330
4000	911.681	2338.863	1589.436	2997.709	466.723	2770.215	-36.175
4100	912.587	2361.386	1607.990	3088.923	463.626	2827.841	-36.026
4200	913.433	2383.388	1626.191	3180.224	460.227	2885.539	-35.886
4300	914.223	2404.891	1644.052	3271.607	456.512	2943.243	-35.753
4400	914.962	2425.917	1661.583	3363.067	452.491	3001.117	-35.627
4500	915.654	2446.486	1678.798	3454.598	448.175	3059.137	-35.509
4600	916.304	2466.619	1695.706	3546.196	443.519	3117.262	-35.397
4700	916.914	2486.331	1712.319	3637.858	438.536	3175.392	-35.290
4800	917.488	2505.642	1728.646	3729.578	433.268	3233.724	-35.189
4900	918.028	2524.565	1744.697	3821.354	427.648	3292.050	-35.093
5000	918.537	2543.117	1760.480	3913.183	421.759	3350.659	-35.003

3.195. Naphth[2,3-*l*]acephenanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-73-5
Point Group: C₁

Length: 15.25 Å
Width: 10.15 Å
Breadth: 4.656 Å
L/B Ratio: 1.503

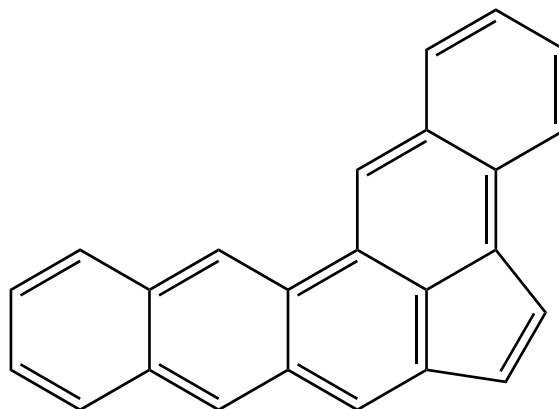
Cartesian coordinates:

C	3.9220	-1.3038	-0.0096	C	-0.7981	0.4856	0.0249	H	-5.6285	1.2634	0.3513
C	2.8867	-0.3231	-0.0470	C	-1.5646	1.6775	0.1981	H	-3.5250	2.5559	0.4100
C	3.4715	0.9709	-0.2428	C	-0.8996	2.9507	0.2535	H	-5.4955	-2.9547	-0.5161
C	4.9205	0.7490	-0.3742	C	0.4377	3.0284	0.0868	H	-6.7921	-0.9036	-0.0276
C	5.1830	-0.5793	-0.2396	C	0.6549	0.5709	0.0405	H	-3.0132	-2.8847	-0.6177
C	-5.0645	0.3483	0.1389	C	1.2438	1.8432	-0.0373	H	-0.9531	-1.6250	-0.4510
C	-2.9537	1.6325	0.2520	C	2.6546	2.0543	-0.2075	H	-1.5074	3.8511	0.3998
C	-3.6381	0.4217	0.0823	C	1.5320	-0.5764	0.1299	H	0.9427	4.0017	0.0708
C	-4.9547	-2.0176	-0.3482	C	3.5864	-2.6065	0.2431	H	3.0407	3.0753	-0.3032
C	-5.7000	-0.8386	-0.0694	C	2.2193	-2.8952	0.4774	H	4.3357	-3.4026	0.2826
C	-3.5939	-1.9802	-0.4041	C	1.2329	-1.9348	0.4334	H	1.9454	-3.9297	0.7132
C	-2.8943	-0.7530	-0.1804	H	5.6354	1.5505	-0.5482	H	0.2000	-2.2301	0.6610
C	-1.4925	-0.6975	-0.2124	H	6.1535	-1.0692	-0.2848				

Table 3.195: Table of thermodynamic data as a function of temperature for Naphth[2,3-*l*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.827	489.969	489.969	∞
100	97.493	335.264	722.089	-38.683	513.347	552.614	-288.650
200	193.322	430.526	552.488	-24.392	500.955	596.820	-155.870
250	249.460	479.649	532.982	-13.333	495.138	621.460	-129.844
298.15	304.220	528.281	528.281	0.000	489.969	646.271	-113.222
300	306.297	530.169	528.287	0.565	489.779	647.240	-112.692
350	360.884	581.528	532.218	17.258	485.026	673.870	-100.568
400	411.426	633.067	541.605	36.585	480.906	701.128	-91.556
450	457.148	684.215	554.615	58.320	477.342	728.874	-84.604
500	497.971	734.535	570.099	82.218	474.253	757.009	-79.083
600	566.348	831.619	605.668	135.571	469.231	814.058	-70.869
700	620.380	923.138	644.552	195.010	465.552	871.843	-65.056
800	663.710	1008.909	684.795	259.291	463.058	930.059	-60.725
900	699.031	1089.190	725.317	327.486	461.595	988.519	-57.371
1000	728.225	1164.399	765.505	398.894	461.023	1047.104	-54.694
1100	752.617	1234.984	805.010	472.971	461.172	1105.719	-52.505
1200	773.174	1301.377	843.635	549.290	461.920	1164.277	-50.679
1300	790.624	1363.971	881.277	627.503	463.110	1222.764	-49.130
1400	805.529	1423.123	917.887	707.330	464.629	1281.149	-47.799
1500	818.333	1479.146	953.453	788.539	466.406	1339.418	-46.642
1600	829.391	1532.321	987.985	870.938	468.328	1397.555	-45.625
1700	838.989	1582.898	1021.505	954.368	470.333	1455.548	-44.723
1800	847.359	1631.095	1054.042	1038.695	472.353	1513.478	-43.919
1900	854.694	1677.110	1085.634	1123.805	474.364	1571.250	-43.196
2000	861.148	1721.118	1116.316	1209.604	476.317	1628.941	-42.543
2100	866.851	1763.274	1146.127	1296.010	478.144	1686.524	-41.949
2200	871.912	1803.719	1175.104	1382.953	479.847	1744.025	-41.408
2300	876.418	1842.579	1203.286	1470.374	481.418	1801.451	-40.911
2400	880.447	1879.965	1230.707	1558.221	482.798	1858.770	-40.454
2500	884.060	1915.982	1257.402	1646.449	483.997	1916.135	-40.035
2600	887.312	1950.719	1283.404	1735.021	484.982	1973.354	-39.644
2700	890.247	1984.263	1308.744	1823.901	485.759	2030.602	-39.284
2800	892.905	2016.688	1333.452	1913.061	486.303	2087.845	-38.948
2900	895.318	2048.064	1357.556	2002.474	486.590	2145.025	-38.635
3000	897.515	2078.454	1381.082	2092.117	486.659	2202.223	-38.343
3100	899.521	2107.917	1404.055	2181.971	486.440	2259.356	-38.069
3200	901.356	2136.505	1426.500	2272.016	485.971	2316.564	-37.813
3300	903.039	2164.267	1448.438	2362.237	485.236	2373.826	-37.574
3400	904.586	2191.249	1469.890	2452.619	484.210	2431.038	-37.348
3500	906.011	2217.491	1490.877	2543.150	482.898	2488.268	-37.135
3600	907.327	2243.033	1511.417	2633.818	481.319	2545.616	-36.935
3700	908.544	2267.910	1531.528	2724.612	479.445	2603.028	-36.747
3800	909.671	2292.154	1551.227	2815.523	477.254	2660.441	-36.570
3900	910.718	2315.797	1570.529	2906.544	474.781	2717.870	-36.401
4000	911.691	2338.867	1589.451	2997.665	472.012	2775.489	-36.243
4100	912.597	2361.390	1608.005	3088.879	468.916	2833.115	-36.094
4200	913.442	2383.392	1626.206	3180.182	465.517	2890.813	-35.952
4300	914.232	2404.895	1644.066	3271.566	461.803	2948.516	-35.817
4400	914.971	2425.921	1661.597	3363.027	457.783	3006.390	-35.690
4500	915.663	2446.491	1678.811	3454.559	453.468	3064.409	-35.570
4600	916.312	2466.623	1695.720	3546.158	448.813	3122.534	-35.457
4700	916.922	2486.336	1712.332	3637.820	443.831	3180.663	-35.348
4800	917.495	2505.647	1728.659	3729.541	438.563	3238.995	-35.247
4900	918.035	2524.570	1744.710	3821.318	432.944	3297.320	-35.149
5000	918.544	2543.122	1760.493	3913.147	427.056	3355.929	-35.058

3.196. Cyclopenta[fg]pentaphene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 777080-20-3
Point Group: C_s

Length: 16.04 Å
Width: 10.16 Å
Breadth: 3.886 Å
L/B Ratio: 1.578

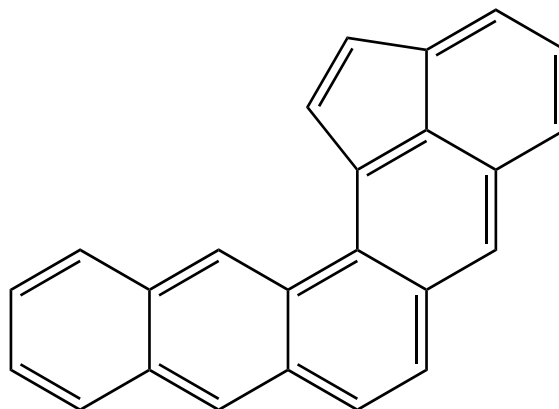
Cartesian coordinates:

C	-1.2864	0.9682	0.0000	C	0.9486	0.0371	0.0000	H	6.2009	-2.4959	0.0000
C	-0.7775	2.3295	0.0000	C	1.4488	1.3830	0.0000	H	7.0720	-0.1776	0.0000
C	-1.9762	3.1845	0.0000	C	0.5537	2.5348	0.0000	H	5.5080	1.7554	0.0000
C	-3.0874	2.3956	0.0000	C	-0.4924	-0.1839	0.0000	H	3.7501	-2.9205	0.0000
C	-2.6811	0.9816	0.0000	C	-1.1614	-1.3977	0.0000	H	3.2145	2.6186	0.0000
C	5.4898	-1.6633	0.0000	C	-2.5787	-1.4366	0.0000	H	1.4392	-2.0531	0.0000
C	5.9886	-0.3359	0.0000	C	-3.3643	-0.2485	0.0000	H	0.9915	3.5392	0.0000
C	5.1304	0.7266	0.0000	C	-4.7840	-0.3447	0.0000	H	-0.5898	-2.3362	0.0000
C	4.1442	-1.8980	0.0000	C	-5.3928	-1.5669	0.0000	H	-5.3702	0.5812	0.0000
C	3.2250	-0.8094	0.0000	C	-4.6179	-2.7543	0.0000	H	-6.4848	-1.6466	0.0000
C	3.7214	0.5131	0.0000	C	-3.2540	-2.6937	0.0000	H	-5.1321	-3.7210	0.0000
C	2.8157	1.5961	0.0000	H	-1.9378	4.2716	0.0000	H	-2.6547	-3.6114	0.0000
C	1.8300	-1.0252	0.0000	H	-4.1264	2.7206	0.0000				

Table 3.196: Table of thermodynamic data as a function of temperature for Cyclopenta[fg]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-45.313	467.390	467.390	∞
100	99.677	338.884	729.183	-39.030	490.420	529.325	-276.485
200	195.061	435.601	558.265	-24.533	478.235	573.085	-149.671
250	250.872	485.075	538.656	-13.395	472.497	597.462	-124.830
298.15	305.393	533.935	533.935	0.000	467.390	622.006	-108.971
300	307.462	535.830	533.941	0.567	467.202	622.964	-108.465
350	361.858	587.353	537.886	17.314	462.501	649.307	-96.902
400	412.248	639.013	547.299	36.685	458.426	676.271	-88.310
450	457.848	690.250	560.342	58.458	454.900	703.717	-81.684
500	498.575	740.638	575.861	82.389	451.844	731.549	-76.423
600	566.823	837.820	611.496	135.795	446.875	787.982	-68.599
700	620.783	929.407	650.439	195.278	443.240	845.144	-63.064
800	664.072	1015.228	690.733	259.597	440.784	902.730	-58.941
900	699.368	1095.551	731.299	327.826	439.356	960.555	-55.748
1000	728.543	1170.794	771.527	399.267	438.817	1018.503	-53.200
1100	752.920	1241.408	811.067	473.375	438.996	1076.477	-51.117
1200	773.461	1307.826	849.724	549.723	439.774	1134.391	-49.378
1300	790.895	1370.444	887.394	627.964	440.992	1192.231	-47.903
1400	805.785	1429.614	924.030	707.818	442.537	1249.969	-46.636
1500	818.574	1485.655	959.621	789.051	444.339	1307.588	-45.533
1600	829.617	1538.845	994.174	871.474	446.285	1365.073	-44.564
1700	839.201	1589.435	1027.714	954.926	448.311	1422.413	-43.705
1800	847.559	1637.644	1060.270	1039.274	450.352	1479.689	-42.939
1900	854.881	1683.670	1091.879	1124.404	452.382	1536.805	-42.249
2000	861.323	1727.687	1122.577	1210.220	454.353	1593.839	-41.626
2100	867.016	1769.852	1152.402	1296.643	456.198	1650.765	-41.060
2200	872.066	1810.304	1181.394	1383.602	457.916	1707.608	-40.543
2300	876.563	1849.170	1209.588	1471.038	459.503	1764.376	-40.069
2400	880.583	1886.563	1237.021	1558.899	460.897	1821.035	-39.633
2500	884.188	1922.584	1263.728	1647.141	462.108	1877.740	-39.232
2600	887.432	1957.327	1289.741	1735.724	463.106	1934.298	-38.860
2700	890.360	1990.875	1315.091	1824.617	463.894	1990.885	-38.515
2800	893.012	2023.304	1339.808	1913.787	464.450	2047.467	-38.195
2900	895.419	2054.683	1363.921	2003.211	464.748	2103.986	-37.896
3000	897.611	2085.077	1387.456	2092.864	464.826	2160.522	-37.617
3100	899.611	2114.543	1410.437	2182.727	464.616	2216.992	-37.355
3200	901.442	2143.133	1432.890	2272.781	464.156	2273.537	-37.111
3300	903.120	2170.898	1454.835	2363.010	463.430	2330.136	-36.882
3400	904.664	2197.882	1476.294	2453.400	462.412	2386.685	-36.666
3500	906.085	2224.127	1497.288	2543.938	461.107	2443.251	-36.463
3600	907.397	2249.671	1517.834	2634.613	459.535	2499.936	-36.272
3700	908.611	2274.550	1537.951	2725.415	457.668	2556.684	-36.093
3800	909.735	2298.796	1557.656	2816.333	455.483	2613.432	-35.923
3900	910.778	2322.440	1576.964	2907.359	453.017	2670.197	-35.763
4000	911.749	2345.511	1595.890	2998.486	450.254	2727.152	-35.612
4100	912.652	2368.036	1614.449	3089.706	447.163	2784.113	-35.469
4200	913.495	2390.039	1632.655	3181.014	443.770	2841.147	-35.334
4300	914.283	2411.543	1650.519	3272.404	440.061	2898.185	-35.205
4400	915.019	2432.571	1668.055	3363.869	436.046	2955.394	-35.084
4500	915.710	2453.142	1685.274	3455.406	431.736	3012.748	-34.970
4600	916.357	2473.275	1702.186	3547.010	427.085	3070.208	-34.863
4700	916.965	2492.989	1718.803	3638.676	422.108	3127.671	-34.759
4800	917.537	2512.300	1735.134	3730.401	416.844	3185.338	-34.663
4900	918.075	2531.225	1751.188	3822.182	411.229	3242.998	-34.570
5000	918.583	2549.778	1766.975	3914.015	405.345	3300.941	-34.484

3.197. Cyclopenta[*pq*]pentaphene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
Point Group: C_s

Length: 15.86 Å
Width: 9.898 Å
Breadth: 3.909 Å
L/B Ratio: 1.603

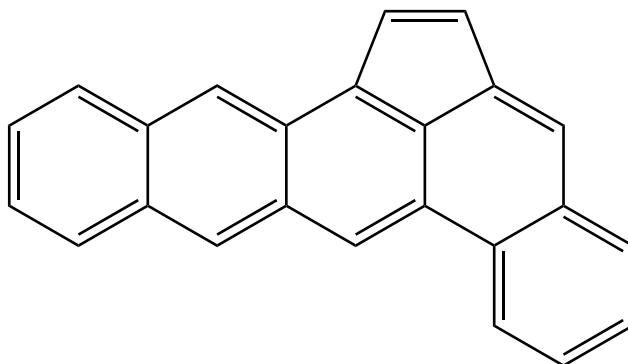
Cartesian coordinates:

C	-4.8874	1.6524	0.0011	C	0.8977	-0.4178	-0.0001	H	5.6619	2.9685	-0.0171
C	-3.5225	1.6686	0.0057	C	3.0236	-1.6335	0.0093	H	6.9208	0.8362	0.0018
C	-2.8134	0.4246	0.0008	C	3.7401	-0.4206	0.0034	H	5.7125	-1.3393	0.0149
C	-3.4428	-0.8130	-0.0072	C	3.0209	0.7932	-0.0072	H	3.1765	2.9650	-0.0233
C	-4.8693	-0.8026	-0.0118	C	1.6100	0.7690	-0.0096	H	3.5792	-2.5798	0.0154
C	-5.5486	0.3891	-0.0079	C	5.1650	-0.3902	0.0066	H	1.0959	1.7384	-0.0203
C	-2.5843	-1.9314	-0.0081	C	5.8263	0.8043	-0.0006	H	1.5491	-3.8233	0.0132
C	-1.2056	-1.7581	-0.0030	C	5.1050	2.0258	-0.0115	H	-0.9169	-3.9251	-0.0003
C	-0.5653	-0.4656	0.0009	C	3.7396	2.0249	-0.0149	H	-3.0179	-2.9390	-0.0120
C	-1.4046	0.6411	0.0058	C	-1.2610	2.1125	0.0167	H	-5.4057	-1.7575	-0.0184
C	-0.3957	-2.9599	0.0011	C	-2.4853	2.7070	0.0161	H	-6.6442	0.3863	-0.0116
C	0.9461	-2.9076	0.0080	H	-2.6998	3.7737	0.0227	H	-5.4765	2.5745	0.0044
C	1.6402	-1.6396	0.0068	H	-0.3064	2.6397	0.0257				

Table 3.197: Table of thermodynamic data as a function of temperature for Cyclopenta[*pq*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.147	489.301	489.301	∞
100	98.364	340.556	729.075	-38.852	512.509	551.247	-287.936
200	194.185	436.410	558.792	-24.476	500.203	594.891	-155.366
250	250.322	485.726	539.222	-13.374	494.429	619.231	-129.379
298.15	305.043	534.508	534.508	0.000	489.301	643.746	-112.779
300	307.118	536.401	534.513	0.566	489.112	644.703	-112.251
350	361.636	587.881	538.454	17.299	484.398	671.019	-100.142
400	412.100	639.516	547.862	36.662	480.314	697.957	-91.142
450	457.744	690.738	560.897	58.428	476.781	725.378	-84.198
500	498.495	741.117	576.409	82.354	473.721	753.186	-78.683
600	566.756	838.286	612.030	135.753	468.745	809.572	-70.478
700	620.702	929.861	650.963	195.229	465.103	866.688	-64.672
800	663.969	1015.671	691.247	259.539	462.638	924.229	-60.345
900	699.243	1095.980	731.805	327.757	461.198	982.011	-56.993
1000	728.401	1171.209	772.024	399.184	460.645	1039.917	-54.319
1100	752.766	1241.809	811.556	473.278	460.810	1097.850	-52.131
1200	773.301	1308.214	850.205	549.610	461.572	1155.724	-50.306
1300	790.733	1370.818	887.868	627.835	462.774	1213.527	-48.759
1400	805.624	1429.977	924.497	707.672	464.303	1271.227	-47.429
1500	818.417	1486.006	960.079	788.890	466.089	1328.811	-46.272
1600	829.465	1539.187	994.626	871.297	468.019	1386.261	-45.256
1700	839.055	1589.767	1028.159	954.734	470.030	1443.567	-44.355
1800	847.419	1637.968	1060.709	1039.067	472.057	1500.811	-43.551
1900	854.747	1683.987	1092.311	1124.184	474.074	1557.895	-42.829
2000	861.196	1727.997	1123.003	1209.988	476.032	1614.898	-42.176
2100	866.895	1770.155	1152.823	1296.398	477.864	1671.793	-41.583
2200	871.952	1810.602	1181.809	1383.345	479.570	1728.606	-41.041
2300	876.455	1849.463	1209.998	1470.770	481.146	1785.344	-40.546
2400	880.481	1886.852	1237.427	1558.620	482.529	1841.974	-40.089
2500	884.091	1922.869	1264.128	1646.852	483.731	1898.651	-39.669
2600	887.341	1957.608	1290.136	1735.427	484.720	1955.180	-39.279
2700	890.274	1991.153	1315.482	1824.310	485.499	2011.739	-38.919
2800	892.930	2023.579	1340.196	1913.472	486.046	2068.293	-38.584
2900	895.341	2054.956	1364.305	2002.888	486.336	2124.785	-38.271
3000	897.537	2085.347	1387.835	2092.533	486.406	2181.294	-37.979
3100	899.541	2114.810	1410.813	2182.389	486.190	2237.737	-37.705
3200	901.375	2143.398	1433.262	2272.436	485.723	2294.256	-37.449
3300	903.057	2171.161	1455.204	2362.659	484.990	2350.828	-37.210
3400	904.603	2198.144	1476.660	2453.043	483.966	2407.350	-36.984
3500	906.028	2224.387	1497.651	2543.575	482.655	2463.891	-36.771
3600	907.342	2249.929	1518.194	2634.245	481.078	2520.550	-36.571
3700	908.558	2274.806	1538.309	2725.040	479.205	2577.272	-36.384
3800	909.685	2299.051	1558.010	2815.953	477.015	2633.995	-36.206
3900	910.731	2322.694	1577.316	2906.975	474.544	2690.734	-36.038
4000	911.703	2345.764	1596.240	2998.097	471.776	2747.664	-35.880
4100	912.609	2368.288	1614.797	3089.313	468.681	2804.600	-35.730
4200	913.453	2390.290	1633.000	3180.617	465.284	2861.608	-35.589
4300	914.243	2411.793	1650.862	3272.002	461.571	2918.621	-35.453
4400	914.981	2432.819	1668.396	3363.464	457.551	2975.806	-35.327
4500	915.672	2453.390	1685.613	3454.997	453.238	3033.135	-35.207
4600	916.321	2473.522	1702.523	3546.597	448.584	3090.570	-35.094
4700	916.931	2493.235	1719.138	3638.260	443.602	3148.009	-34.985
4800	917.504	2512.546	1735.466	3729.982	438.335	3205.651	-34.884
4900	918.043	2531.470	1751.519	3821.759	432.717	3263.286	-34.786
5000	918.552	2550.022	1767.304	3913.589	426.830	3321.205	-34.696

3.198. Benzo[*a*]cyclopenta[*de*]naphthacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908068-87-1
Point Group: C_s

Length: 16.14 Å
Width: 10.03 Å
Breadth: 3.885 Å
L/B Ratio: 1.610

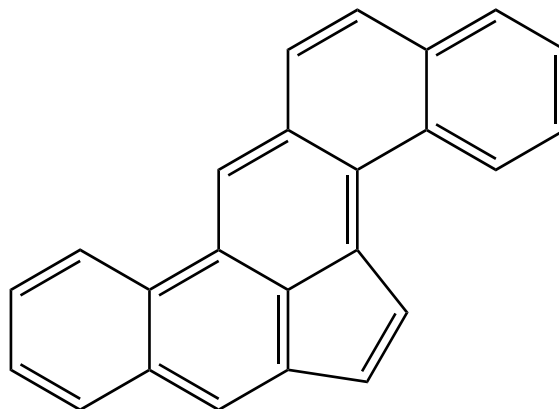
Cartesian coordinates:

C	3.1769	2.2009	0.0000	C	-0.0522	-1.5574	0.0000	H	-6.7014	1.9860	0.0000
C	2.8223	0.8441	0.0000	C	-2.5094	-1.2574	0.0000	H	-7.0395	-0.4650	0.0000
C	3.8358	-0.1428	0.0000	C	-3.6110	-0.4082	0.0000	H	-5.0907	-2.0095	0.0000
C	5.1807	0.2647	0.0000	C	-3.4158	1.0034	0.0000	H	-4.4082	2.9453	0.0000
C	5.5113	1.6075	0.0000	C	-2.1267	1.5255	0.0000	H	-2.6517	-2.3451	0.0000
C	4.5071	2.5791	0.0000	C	-4.9516	-0.9225	0.0000	H	-1.9829	2.6134	0.0000
C	3.5320	-1.5667	0.0000	C	-6.0153	-0.0781	0.0000	H	0.4233	2.3419	0.0000
C	2.2413	-1.9575	0.0000	C	-5.8202	1.3363	0.0000	H	4.3619	-2.2819	0.0000
C	1.1957	-0.9495	0.0000	C	-4.5677	1.8611	0.0000	H	5.9726	-0.4936	0.0000
C	1.4239	0.4394	0.0000	C	0.1847	-3.0085	0.0000	H	6.5627	1.9135	0.0000
C	0.3083	1.2490	0.0000	C	1.5277	-3.2451	0.0000	H	4.7765	3.6404	0.0000
C	-1.0030	0.6812	0.0000	H	-0.6144	-3.7476	0.0000	H	2.3781	2.9550	0.0000
C	-1.2079	-0.7373	0.0000	H	2.0290	-4.2104	0.0000				

Table 3.198: Table of thermodynamic data as a function of temperature for Benzo[*a*]cyclopenta[*de*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.170	480.963	480.963	∞
100	99.221	337.239	726.642	-38.940	504.083	543.153	-283.708
200	194.608	433.631	556.081	-24.490	491.851	587.096	-153.330
250	250.435	483.005	536.504	-13.375	486.091	611.573	-127.779
298.15	304.978	531.790	531.790	0.000	480.963	636.219	-111.461
300	307.049	533.683	531.795	0.566	480.775	637.181	-110.941
350	361.476	585.144	535.735	17.293	476.054	663.633	-99.040
400	411.903	636.755	545.139	36.646	471.961	690.709	-90.195
450	457.540	687.953	558.169	58.403	468.419	718.269	-83.373
500	498.303	738.312	573.673	82.319	465.348	746.216	-77.955
600	566.609	835.449	609.281	135.701	460.355	802.885	-69.896
700	620.610	927.006	648.199	195.164	456.701	860.285	-64.194
800	663.928	1012.806	688.472	259.468	454.229	918.112	-59.945
900	699.246	1093.113	729.019	327.684	452.788	976.181	-56.655
1000	728.437	1168.344	769.231	399.113	452.237	1034.373	-54.029
1100	752.826	1238.949	808.756	473.212	452.407	1092.592	-51.882
1200	773.378	1305.360	847.401	549.551	453.175	1150.752	-50.090
1300	790.820	1367.970	885.060	627.784	454.386	1208.840	-48.571
1400	805.717	1427.136	921.686	707.630	455.924	1266.825	-47.265
1500	818.512	1483.172	957.267	788.858	457.719	1324.692	-46.129
1600	829.561	1536.359	991.812	871.274	459.659	1382.426	-45.131
1700	839.149	1586.945	1025.344	954.721	461.680	1440.014	-44.245
1800	847.511	1635.152	1057.894	1039.064	463.716	1497.540	-43.457
1900	854.837	1681.175	1089.496	1124.189	465.741	1554.906	-42.746
2000	861.282	1725.189	1120.189	1210.002	467.708	1612.189	-42.105
2100	866.978	1767.352	1150.009	1296.420	469.549	1669.365	-41.522
2200	872.031	1807.803	1178.996	1383.376	471.263	1726.458	-40.990
2300	876.531	1846.667	1207.186	1470.808	472.847	1783.475	-40.503
2400	880.553	1884.059	1234.615	1558.666	474.237	1840.385	-40.054
2500	884.160	1920.079	1261.317	1646.905	475.446	1897.341	-39.642
2600	887.406	1954.821	1287.326	1735.486	476.441	1954.149	-39.259
2700	890.336	1988.368	1312.673	1824.375	477.227	2010.987	-38.904
2800	892.989	2020.796	1337.387	1913.544	477.780	2067.820	-38.575
2900	895.397	2052.175	1361.497	2002.965	478.075	2124.589	-38.267
3000	897.590	2082.568	1385.029	2092.616	478.151	2181.376	-37.980
3100	899.592	2112.032	1408.008	2182.477	477.940	2238.097	-37.711
3200	901.423	2140.623	1430.457	2272.529	477.478	2294.894	-37.460
3300	903.103	2168.387	1452.400	2362.756	476.750	2351.744	-37.224
3400	904.647	2195.371	1473.857	2453.145	475.730	2408.543	-37.002
3500	906.069	2221.615	1494.849	2543.682	474.424	2465.361	-36.793
3600	907.382	2247.158	1515.393	2634.355	472.850	2522.297	-36.597
3700	908.596	2272.036	1535.508	2725.155	470.982	2579.296	-36.412
3800	909.721	2296.282	1555.211	2816.071	468.796	2636.296	-36.238
3900	910.766	2319.926	1574.517	2907.096	466.328	2693.312	-36.072
4000	911.737	2342.997	1593.442	2998.222	463.564	2750.518	-35.917
4100	912.641	2365.522	1611.999	3089.442	460.472	2807.731	-35.770
4200	913.484	2387.524	1630.203	3180.748	457.078	2865.016	-35.631
4300	914.272	2409.028	1648.066	3272.137	453.368	2922.306	-35.498
4400	915.009	2430.056	1665.601	3363.601	449.351	2979.766	-35.374
4500	915.700	2450.626	1682.818	3455.137	445.040	3037.372	-35.256
4600	916.348	2470.760	1699.729	3546.740	440.389	3095.083	-35.145
4700	916.956	2490.473	1716.345	3638.405	435.410	3152.798	-35.039
4800	917.528	2509.784	1732.674	3730.130	430.146	3210.717	-34.939
4900	918.067	2528.709	1748.727	3821.910	424.530	3268.628	-34.843
5000	918.575	2547.261	1764.513	3913.742	418.645	3326.823	-34.754

3.199. Dibenz[*e,l*]aceanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 777080-21-4
Point Group: C_s

Length: 15.79 Å
Width: 9.769 Å
Breadth: 3.908 Å
L/B Ratio: 1.617

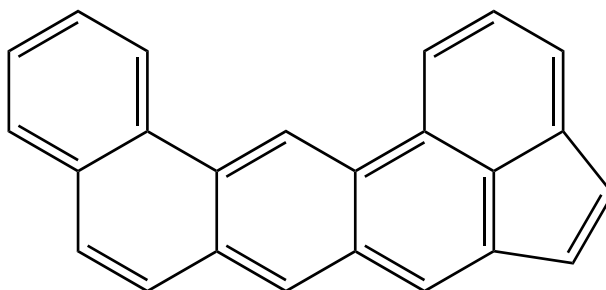
Cartesian coordinates:

C	5.0448	-0.5475	-0.0023	C	-0.5109	-1.0399	0.0038	H	-6.7808	-0.2918	-0.0047
C	3.6378	-0.6239	-0.0005	C	-1.6954	2.5050	0.0071	H	-5.6527	1.9249	0.0126
C	2.8889	0.5750	-0.0023	C	-3.0379	2.3853	0.0107	H	-2.9723	-2.2564	-0.0280
C	3.5571	1.8121	-0.0056	C	-3.6548	1.0864	0.0050	H	-5.4126	-2.3678	-0.0269
C	4.9356	1.8620	-0.0072	C	-2.8644	-0.0809	-0.0029	H	-3.6864	3.2691	0.0167
C	5.6821	0.6760	-0.0056	C	-5.0614	1.0019	0.0049	H	-1.2226	3.4946	0.0091
C	1.4411	0.5095	-0.0006	C	-5.6883	-0.2244	-0.0051	H	0.9382	2.6053	-0.0003
C	0.8735	-0.7586	0.0022	C	-4.9160	-1.3918	-0.0169	H	3.6201	-2.8235	0.0055
C	1.6454	-1.9822	0.0052	C	-3.5389	-1.3186	-0.0163	H	2.9561	2.7321	-0.0067
C	2.9961	-1.9231	0.0036	C	-0.5959	-2.5155	0.0103	H	5.4523	2.8273	-0.0097
C	0.5439	1.5786	0.0001	C	0.6504	-3.0611	0.0105	H	6.7759	0.7265	-0.0070
C	-0.8384	1.3450	0.0019	H	-1.5281	-3.0812	0.0158	H	5.6315	-1.4735	-0.0009
C	-1.4125	0.0326	0.0007	H	0.9076	-4.1183	0.0146				

Table 3.199: Table of thermodynamic data as a function of temperature for Dibenz[*e,l*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-45.116	466.847	466.847	∞
100	99.147	338.247	726.659	-38.841	490.066	529.035	-276.334
200	194.081	434.427	556.547	-24.424	477.801	572.886	-149.619
250	249.748	483.666	537.023	-13.339	472.010	597.328	-124.802
298.15	304.203	532.321	532.321	0.000	466.847	621.945	-108.960
300	306.271	534.209	532.327	0.565	466.657	622.906	-108.455
350	360.676	585.548	536.257	17.252	461.897	649.334	-96.906
400	411.125	637.053	545.639	36.566	457.764	676.392	-88.326
450	456.804	688.163	558.641	58.285	454.184	703.940	-81.710
500	497.612	738.446	574.116	82.165	451.078	731.879	-76.457
600	565.998	835.464	609.661	135.482	446.020	788.540	-68.647
700	620.052	926.931	648.521	194.887	442.307	845.943	-63.124
800	663.405	1012.660	688.739	259.137	439.782	903.782	-59.010
900	698.748	1092.907	729.238	327.302	438.289	961.868	-55.824
1000	727.961	1168.086	769.404	398.682	437.690	1020.083	-53.283
1100	752.372	1238.647	808.888	472.735	437.813	1078.331	-51.205
1200	772.947	1305.019	847.495	549.029	438.537	1136.523	-49.471
1300	790.412	1367.596	885.119	627.220	439.706	1194.647	-48.001
1400	805.333	1426.732	921.713	707.027	441.204	1252.670	-46.737
1500	818.151	1482.742	957.264	788.217	442.962	1310.579	-45.637
1600	829.222	1535.907	991.782	870.599	444.867	1368.357	-44.671
1700	838.832	1586.473	1025.289	954.013	446.855	1425.992	-43.814
1800	847.214	1634.662	1057.815	1038.324	448.861	1483.565	-43.051
1900	854.558	1680.670	1089.395	1123.421	450.857	1540.981	-42.364
2000	861.022	1724.671	1120.067	1209.207	452.797	1598.316	-41.743
2100	866.734	1766.821	1149.868	1295.600	454.613	1655.544	-41.179
2200	871.802	1807.261	1178.837	1382.532	456.303	1712.691	-40.664
2300	876.316	1846.115	1207.010	1469.942	457.865	1769.763	-40.192
2400	880.351	1883.498	1234.423	1557.779	459.235	1826.729	-39.757
2500	883.970	1919.510	1261.111	1645.999	460.424	1883.741	-39.358
2600	887.227	1954.245	1287.106	1734.561	461.401	1940.606	-38.986
2700	890.168	1987.785	1312.439	1823.434	462.169	1997.502	-38.643
2800	892.830	2020.207	1337.141	1912.586	462.706	2054.393	-38.324
2900	895.248	2051.581	1361.239	2001.991	462.986	2111.222	-38.026
3000	897.449	2081.969	1384.759	2091.628	463.047	2168.068	-37.749
3100	899.458	2111.429	1407.728	2181.475	462.822	2224.849	-37.488
3200	901.296	2140.015	1430.167	2271.514	462.347	2281.707	-37.244
3300	902.983	2167.776	1452.100	2361.729	461.606	2338.617	-37.016
3400	904.533	2194.756	1473.548	2452.106	460.575	2395.478	-36.801
3500	905.961	2220.997	1494.531	2542.631	459.258	2452.358	-36.599
3600	907.279	2246.537	1515.067	2633.294	457.674	2509.356	-36.409
3700	908.498	2271.413	1535.174	2724.084	455.795	2566.417	-36.231
3800	909.627	2295.656	1554.869	2814.991	453.599	2623.480	-36.061
3900	910.676	2319.298	1574.168	2906.007	451.122	2680.559	-35.901
4000	911.651	2342.366	1593.085	2997.124	448.349	2737.828	-35.752
4100	912.559	2364.889	1611.636	3088.335	445.249	2795.104	-35.609
4200	913.406	2386.889	1629.834	3179.633	441.847	2852.452	-35.475
4300	914.197	2408.392	1647.691	3271.014	438.129	2909.805	-35.346
4400	914.937	2429.417	1665.219	3362.471	434.105	2967.330	-35.226
4500	915.631	2449.986	1682.431	3454.000	429.787	3024.999	-35.113
4600	916.281	2470.118	1699.336	3545.596	425.129	3082.774	-35.005
4700	916.892	2489.830	1715.946	3637.255	420.144	3140.554	-34.903
4800	917.467	2509.140	1732.271	3728.973	414.873	3198.536	-34.806
4900	918.008	2528.063	1748.319	3820.747	409.251	3256.512	-34.714
5000	918.518	2546.615	1764.100	3912.573	403.361	3314.772	-34.628

3.200. Naphth[2,1-*k*]acephenanthrylene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 908068-94-0
Point Group: C_s

Length: 15.27 Å
Width: 9.458 Å
Breadth: 3.888 Å
L/B Ratio: 1.614

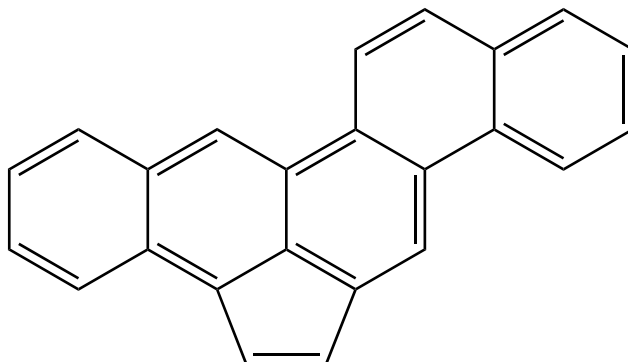
Cartesian coordinates:

C	3.1548	0.1199	0.0000	C	-1.6647	-0.2232	0.0000	H	-6.5570	1.9261	0.0000
C	3.2967	-1.3189	0.0000	C	-1.5388	-1.6314	0.0000	H	-6.2849	-0.5442	0.0000
C	4.7494	-1.5636	0.0000	C	-0.2687	-2.2154	0.0000	H	-2.2681	2.4086	0.0000
C	5.4098	-0.3731	0.0000	C	-0.5109	0.5656	0.0000	H	-4.5596	3.4016	0.0000
C	4.4341	0.7304	0.0000	C	0.7563	-0.0108	0.0000	H	-4.8570	-2.5160	0.0000
C	-5.5568	1.4808	0.0000	C	0.8860	-1.4310	0.0000	H	-2.5967	-3.5400	0.0000
C	-5.4062	0.1108	0.0000	C	2.1833	-2.0843	0.0000	H	-0.1811	-3.3095	0.0000
C	-3.1637	1.7684	0.0000	C	1.9554	0.8062	0.0000	H	-0.6140	1.6649	0.0000
C	-4.4286	2.3147	0.0000	C	4.5019	2.1047	0.0000	H	2.2245	-3.1790	0.0000
C	-2.9873	0.3702	0.0000	C	3.2897	2.8292	0.0000	H	5.4604	2.6320	0.0000
C	-4.1190	-0.4632	0.0000	C	2.0490	2.2153	0.0000	H	3.3407	3.9236	0.0000
C	-3.9548	-1.8936	0.0000	H	5.1873	-2.5598	0.0000	H	1.1281	2.8117	0.0000
C	-2.7234	-2.4512	0.0000	H	6.4869	-0.2176	0.0000				

Table 3.200: Table of thermodynamic data as a function of temperature for Naphth[2,1-*k*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.127	453.482	453.482	∞
100	99.045	339.566	727.908	-38.834	476.708	515.545	-269.288
200	194.000	435.608	557.792	-24.437	464.423	559.272	-146.064
250	249.896	484.854	538.255	-13.350	458.634	583.654	-121.945
298.15	304.494	533.549	533.549	0.000	453.482	608.213	-106.554
300	306.566	535.439	533.555	0.565	453.292	609.172	-106.064
350	361.035	586.829	537.489	17.269	448.549	635.538	-94.847
400	411.493	638.383	546.880	36.601	444.434	662.531	-86.516
450	457.157	689.535	559.895	58.338	440.872	690.011	-80.093
500	497.941	739.854	575.383	82.235	437.784	717.880	-74.995
600	566.282	836.929	610.957	135.583	432.756	774.397	-67.416
700	620.310	928.437	649.844	195.015	429.070	831.652	-62.057
800	663.651	1014.199	690.087	259.290	426.570	889.338	-58.067
900	698.987	1094.475	730.608	327.480	425.102	947.270	-54.977
1000	728.196	1169.679	770.796	398.884	424.526	1005.327	-52.512
1100	752.601	1240.262	810.299	472.959	424.672	1063.413	-50.496
1200	773.169	1306.654	848.924	549.276	425.419	1121.444	-48.814
1300	790.627	1369.248	886.564	627.489	426.610	1179.403	-47.388
1400	805.537	1428.400	923.174	707.317	428.129	1237.260	-46.162
1500	818.345	1484.424	958.740	788.527	429.907	1295.002	-45.095
1600	829.406	1537.601	993.271	870.928	431.831	1352.611	-44.157
1700	839.006	1588.178	1026.790	954.359	433.837	1410.075	-43.325
1800	847.378	1636.376	1059.328	1038.688	435.859	1467.478	-42.584
1900	854.713	1682.393	1090.919	1123.801	437.872	1524.722	-41.917
2000	861.168	1726.401	1121.601	1209.601	439.827	1581.884	-41.314
2100	866.871	1768.559	1151.411	1296.009	441.656	1638.938	-40.766
2200	871.931	1809.005	1180.389	1382.954	443.360	1695.911	-40.265
2300	876.437	1847.865	1208.570	1470.377	444.934	1752.809	-39.807
2400	880.465	1885.252	1235.992	1558.226	446.316	1809.599	-39.384
2500	884.078	1921.269	1262.687	1646.456	447.516	1866.436	-38.996
2600	887.329	1956.008	1288.689	1735.029	448.503	1923.125	-38.635
2700	890.264	1989.552	1314.029	1823.911	449.281	1979.844	-38.302
2800	892.921	2021.977	1338.737	1913.073	449.828	2036.559	-37.992
2900	895.333	2053.354	1362.841	2002.487	450.116	2093.210	-37.702
3000	897.530	2083.745	1386.367	2092.132	450.186	2149.879	-37.432
3100	899.535	2113.208	1409.341	2181.987	449.969	2206.482	-37.178
3200	901.369	2141.796	1431.786	2272.033	449.502	2263.162	-36.942
3300	903.052	2169.559	1453.724	2362.256	448.768	2319.894	-36.720
3400	904.599	2196.541	1475.177	2452.639	447.743	2376.577	-36.511
3500	906.023	2222.784	1496.164	2543.171	446.432	2433.278	-36.314
3600	907.339	2248.326	1516.704	2633.840	444.854	2490.097	-36.130
3700	908.555	2273.203	1536.815	2724.636	442.982	2546.979	-35.956
3800	909.682	2297.448	1556.514	2815.548	440.791	2603.863	-35.792
3900	910.728	2321.091	1575.817	2906.569	438.320	2660.762	-35.636
4000	911.701	2344.161	1594.738	2997.691	435.552	2717.852	-35.491
4100	912.606	2366.684	1613.292	3088.907	432.456	2774.949	-35.353
4200	913.451	2388.686	1631.493	3180.211	429.059	2832.117	-35.222
4300	914.241	2410.190	1649.353	3271.596	425.346	2889.291	-35.097
4400	914.979	2431.216	1666.885	3363.057	421.326	2946.635	-34.980
4500	915.671	2451.786	1684.099	3454.590	417.012	3004.125	-34.870
4600	916.320	2471.919	1701.008	3546.190	412.358	3061.720	-34.766
4700	916.929	2491.632	1717.621	3637.853	407.377	3119.319	-34.667
4800	917.502	2510.942	1733.948	3729.574	402.110	3177.122	-34.573
4900	918.042	2529.866	1749.999	3821.352	396.491	3234.917	-34.484
5000	918.551	2548.418	1765.782	3913.182	390.604	3292.997	-34.401

3.201. Benzo[*b*]cyclopenta[*qr*]chrysene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 777080-22-5
Point Group: C_s

Length: 16.13 Å
Width: 9.779 Å
Breadth: 3.888 Å
L/B Ratio: 1.650

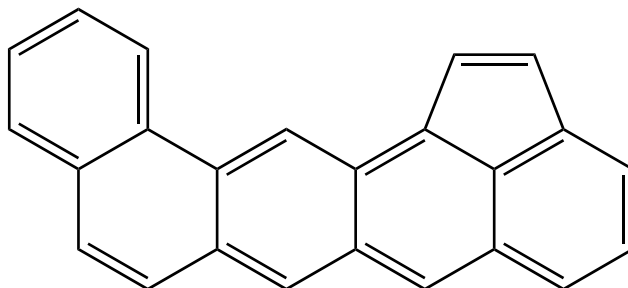
Cartesian coordinates:

C	-5.0123	-1.3951	0.0000	C	0.5933	-0.5008	0.0000	H	1.3112	-2.5324	0.0000
C	-3.6139	-1.1613	0.0000	C	1.5952	-1.4697	0.0000	H	-1.9345	2.5804	0.0000
C	-3.1262	0.1605	0.0000	C	2.9531	-1.0903	0.0000	H	3.6678	-3.1477	0.0000
C	-4.0612	1.2274	0.0000	C	3.3574	0.2805	0.0000	H	6.0681	-2.5242	0.0000
C	-5.4098	0.9814	0.0000	C	2.3512	1.2543	0.0000	H	6.7530	-0.1455	0.0000
C	-5.8921	-0.3436	0.0000	C	3.9725	-2.0948	0.0000	H	5.0356	1.6595	0.0000
C	-1.7062	0.3956	0.0000	C	5.2911	-1.7527	0.0000	H	-3.0997	-3.2774	0.0000
C	-0.8403	-0.7055	0.0000	C	5.6849	-0.3866	0.0000	H	-0.6334	-2.8597	0.0000
C	-1.3579	-2.0318	0.0000	C	4.7475	0.6021	0.0000	H	-3.6800	2.2597	0.0000
C	-2.6999	-2.2569	0.0000	C	2.3138	2.7250	0.0000	H	-6.1242	1.8112	0.0000
C	-1.2073	1.7550	0.0000	C	1.0162	3.1441	0.0000	H	-6.9724	-0.5212	0.0000
C	0.1293	1.9689	0.0000	H	3.2068	3.3475	0.0000	H	-5.3770	-2.4287	0.0000
C	1.0157	0.8294	0.0000	H	0.6543	4.1699	0.0000				

Table 3.201: Table of thermodynamic data as a function of temperature for Benzo[*b*]cyclopenta[*qr*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.358	469.355	469.355	∞
100	100.268	338.591	729.098	-39.051	492.364	531.299	-277.516
200	195.125	435.548	558.158	-24.522	480.211	575.072	-150.190
250	250.748	485.015	538.560	-13.386	474.471	599.451	-125.246
298.15	305.153	533.842	533.842	0.000	469.355	623.999	-109.320
300	307.219	535.736	533.848	0.566	469.166	624.957	-108.812
350	361.555	587.216	537.789	17.299	464.452	651.306	-97.200
400	411.926	638.834	547.196	36.655	460.361	678.277	-88.572
450	457.527	690.033	560.228	58.412	456.819	705.733	-81.918
500	498.263	740.388	575.735	82.327	453.747	733.577	-76.635
600	566.529	837.514	611.344	135.702	448.748	790.038	-68.778
700	620.496	929.056	650.261	195.156	445.084	847.233	-63.220
800	663.784	1014.840	690.531	259.447	442.600	904.856	-59.080
900	699.078	1095.128	731.075	327.648	441.142	962.722	-55.874
1000	728.253	1170.340	771.282	399.059	440.574	1020.713	-53.315
1100	752.633	1240.928	810.801	473.139	440.725	1078.734	-51.224
1200	773.182	1307.321	849.439	549.458	441.474	1136.697	-49.478
1300	790.625	1369.916	887.092	627.672	442.665	1194.590	-47.998
1400	805.526	1429.067	923.711	707.499	444.183	1252.380	-46.726
1500	818.327	1485.090	959.286	788.707	445.960	1310.055	-45.619
1600	829.383	1538.266	993.824	871.106	447.882	1367.598	-44.647
1700	838.980	1588.841	1027.350	954.535	449.885	1424.996	-43.784
1800	847.351	1637.038	1059.893	1038.861	451.905	1482.332	-43.015
1900	854.685	1683.053	1091.489	1123.971	453.915	1539.510	-42.323
2000	861.139	1727.060	1122.176	1209.769	455.867	1596.606	-41.698
2100	866.842	1769.216	1151.991	1296.174	457.693	1653.595	-41.130
2200	871.902	1809.661	1180.972	1383.116	459.395	1710.502	-40.612
2300	876.409	1848.520	1209.156	1470.536	460.965	1767.334	-40.137
2400	880.438	1885.906	1236.580	1558.382	462.345	1824.059	-39.699
2500	884.052	1921.922	1263.278	1646.609	463.542	1880.830	-39.297
2600	887.304	1956.659	1289.282	1735.180	464.527	1937.454	-38.923
2700	890.239	1990.203	1314.625	1824.060	465.302	1994.109	-38.578
2800	892.897	2022.627	1339.335	1913.219	465.846	2050.758	-38.257
2900	895.311	2054.003	1363.441	2002.631	466.133	2107.344	-37.957
3000	897.508	2084.393	1386.968	2092.274	466.200	2163.948	-37.677
3100	899.514	2113.855	1409.944	2182.126	465.981	2220.487	-37.414
3200	901.349	2142.443	1432.390	2272.171	465.511	2277.101	-37.169
3300	903.033	2170.205	1454.329	2362.391	464.776	2333.769	-36.940
3400	904.580	2197.187	1475.783	2452.773	463.750	2390.387	-36.723
3500	906.006	2223.429	1496.771	2543.303	462.437	2447.024	-36.519
3600	907.322	2248.971	1517.312	2633.970	460.857	2503.778	-36.328
3700	908.539	2273.847	1537.425	2724.764	458.983	2560.596	-36.148
3800	909.666	2298.092	1557.125	2815.675	456.791	2617.415	-35.978
3900	910.713	2321.734	1576.428	2906.695	454.317	2674.251	-35.817
4000	911.686	2344.804	1595.350	2997.815	451.548	2731.276	-35.666
4100	912.593	2367.327	1613.905	3089.030	448.451	2788.308	-35.523
4200	913.438	2389.329	1632.107	3180.332	445.052	2845.412	-35.387
4300	914.228	2410.832	1649.968	3271.715	441.338	2902.522	-35.258
4400	914.967	2431.858	1667.500	3363.175	437.317	2959.802	-35.137
4500	915.659	2452.428	1684.715	3454.707	433.002	3017.227	-35.022
4600	916.308	2472.560	1701.624	3546.306	428.347	3074.759	-34.914
4700	916.918	2492.273	1718.237	3637.967	423.364	3132.294	-34.811
4800	917.492	2511.583	1734.565	3729.688	418.096	3190.032	-34.714
4900	918.032	2530.507	1750.616	3821.465	412.477	3247.764	-34.621
5000	918.541	2549.059	1766.400	3913.294	406.588	3305.779	-34.535

3.202. Benzo[*a*]cyclopenta[*mn*]naphthacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908069-02-3
Point Group: C_s

Length: 15.77 Å
Width: 9.326 Å
Breadth: 3.887 Å
L/B Ratio: 1.691

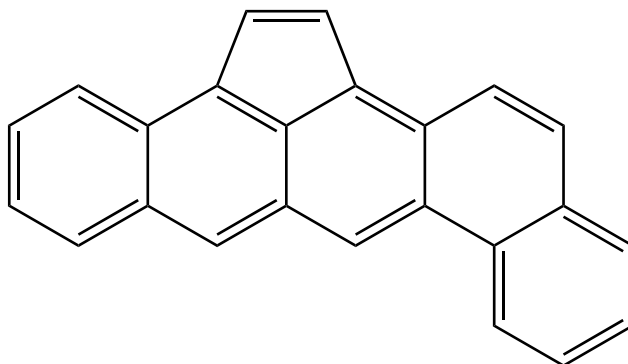
Cartesian coordinates:

C	3.2909	1.7968	0.0000	C	0.6159	0.6681	0.0000	H	-6.2943	1.4822	0.0000
C	3.0752	0.4082	0.0000	C	-2.1410	-1.9031	0.0000	H	-6.7114	-0.9576	0.0000
C	4.1822	-0.4571	0.0000	C	-3.2891	-1.1142	0.0000	H	-4.8770	-2.6136	0.0000
C	5.4822	0.0761	0.0000	C	-3.0920	0.2724	0.0000	H	-2.2245	-2.9964	0.0000
C	5.6744	1.4447	0.0000	C	-1.8472	0.9148	0.0000	H	0.1783	-3.2088	0.0000
C	4.5741	2.3085	0.0000	C	-4.6615	-1.5397	0.0000	H	0.7407	1.7632	0.0000
C	3.9778	-1.8877	0.0000	C	-5.6694	-0.6187	0.0000	H	2.5837	-3.4987	0.0000
C	2.7371	-2.4132	0.0000	C	-5.4394	0.7992	0.0000	H	4.8653	-2.5310	0.0000
C	1.5627	-1.5677	0.0000	C	-4.1557	1.2447	0.0000	H	6.3425	-0.6029	0.0000
C	1.7278	-0.1439	0.0000	C	-3.4804	2.5526	0.0000	H	6.6884	1.8578	0.0000
C	0.3008	-2.1180	0.0000	C	-2.1302	2.3579	0.0000	H	4.7336	3.3916	0.0000
C	-0.8627	-1.3010	0.0000	H	-4.0103	3.5026	0.0000	H	2.4153	2.4643	0.0000
C	-0.6908	0.1219	0.0000	H	-1.3547	3.1215	0.0000				

Table 3.202: Table of thermodynamic data as a function of temperature for Benzo[*a*]cyclopenta[*mn*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.324	488.856	488.856	∞
100	99.392	340.360	730.380	-39.002	511.914	550.672	-287.635
200	194.890	436.802	559.521	-24.544	499.690	594.300	-155.212
250	251.004	486.272	539.899	-13.407	493.951	618.617	-129.250
298.15	305.721	535.173	535.173	0.000	488.856	643.103	-112.667
300	307.797	537.071	535.179	0.568	488.668	644.058	-112.138
350	362.310	588.655	539.129	17.334	483.988	670.338	-100.040
400	412.762	640.380	548.554	36.730	479.937	697.235	-91.048
450	458.388	691.679	561.613	58.530	476.438	724.611	-84.109
500	499.116	742.125	577.150	82.487	473.409	752.370	-78.598
600	567.324	839.402	612.826	135.946	468.492	808.650	-70.398
700	621.219	931.061	651.810	195.475	464.904	865.649	-64.594
800	664.441	1016.937	692.143	259.835	462.489	923.067	-60.269
900	699.675	1097.299	732.745	328.098	461.094	980.720	-56.918
1000	728.798	1172.571	773.005	399.567	460.583	1038.491	-54.244
1100	753.130	1243.208	812.573	473.699	460.785	1096.286	-52.057
1200	773.636	1309.643	851.255	550.065	461.582	1154.019	-50.232
1300	791.041	1372.273	888.948	628.323	462.816	1211.678	-48.685
1400	805.908	1431.454	925.604	708.189	464.375	1269.231	-47.355
1500	818.678	1487.502	961.212	789.434	466.188	1326.666	-46.198
1600	829.706	1540.699	995.782	871.867	468.144	1383.966	-45.181
1700	839.277	1591.293	1029.336	955.327	470.178	1441.120	-44.279
1800	847.624	1639.507	1061.906	1039.681	472.226	1498.211	-43.476
1900	854.938	1685.536	1093.526	1124.817	474.262	1555.141	-42.753
2000	861.373	1729.555	1124.235	1210.640	476.239	1611.988	-42.100
2100	867.060	1771.722	1154.071	1297.067	478.088	1668.727	-41.506
2200	872.105	1812.177	1183.072	1384.030	479.810	1725.383	-40.965
2300	876.598	1851.044	1211.275	1471.470	481.401	1781.963	-40.469
2400	880.614	1888.438	1238.716	1559.334	482.798	1838.435	-40.012
2500	884.216	1924.461	1265.430	1647.579	484.013	1894.952	-39.592
2600	887.458	1959.205	1291.449	1736.165	485.013	1951.322	-39.202
2700	890.384	1992.754	1316.806	1825.060	485.804	2007.722	-38.841
2800	893.033	2025.184	1341.529	1914.233	486.362	2064.115	-38.506
2900	895.438	2056.564	1365.647	2003.658	486.661	2120.446	-38.193
3000	897.629	2086.958	1389.187	2093.313	486.741	2176.794	-37.901
3100	899.628	2116.424	1412.173	2183.178	486.533	2233.076	-37.626
3200	901.457	2145.016	1434.630	2273.233	486.075	2289.433	-37.370
3300	903.134	2172.781	1456.580	2363.464	485.350	2345.844	-37.131
3400	904.677	2199.765	1478.043	2453.855	484.333	2402.204	-36.905
3500	906.097	2226.011	1499.040	2544.395	483.030	2458.582	-36.692
3600	907.408	2251.555	1519.590	2635.071	481.459	2515.079	-36.492
3700	908.621	2276.433	1539.711	2725.874	479.593	2571.638	-36.304
3800	909.745	2300.680	1559.419	2816.793	477.409	2628.198	-36.126
3900	910.788	2324.325	1578.730	2907.820	474.944	2684.775	-35.958
4000	911.758	2347.396	1597.659	2998.948	472.182	2741.541	-35.800
4100	912.661	2369.921	1616.221	3090.169	469.092	2798.314	-35.650
4200	913.503	2391.924	1634.429	3181.478	465.700	2855.159	-35.508
4300	914.290	2413.429	1652.297	3272.868	461.992	2912.008	-35.373
4400	915.027	2434.456	1669.835	3364.334	457.977	2969.029	-35.246
4500	915.716	2455.027	1687.056	3455.872	453.668	3026.194	-35.126
4600	916.363	2475.161	1703.971	3547.476	449.018	3083.465	-35.013
4700	916.971	2494.875	1720.589	3639.143	444.041	3140.741	-34.905
4800	917.543	2514.187	1736.922	3730.869	438.778	3198.219	-34.803
4900	918.081	2533.111	1752.978	3822.650	433.163	3255.690	-34.705
5000	918.588	2551.664	1768.767	3914.484	427.280	3313.445	-34.615

3.203. Benzo[*a*]cyclopenta[*fg*]naphthacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908069-10-3
Point Group: C_s

Length: 16.07 Å
Width: 9.434 Å
Breadth: 3.887 Å
L/B Ratio: 1.704

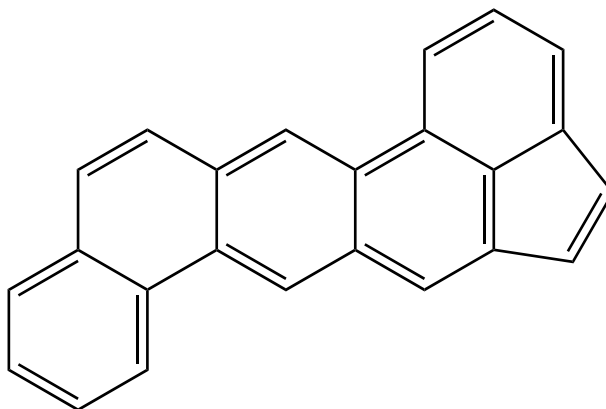
Cartesian coordinates:

C	3.4253	1.9173	0.0000	C	0.6345	1.1779	0.0000	H	-6.4033	2.2924	0.0000
C	3.0255	0.5690	0.0000	C	-1.8529	1.7021	0.0000	H	-6.8430	-0.1426	0.0000
C	4.0146	-0.4299	0.0000	C	-3.1528	1.1855	0.0000	H	-4.9534	-1.7661	0.0000
C	5.3734	-0.0701	0.0000	C	-3.4179	-0.2265	0.0000	H	-4.0809	3.1592	0.0000
C	5.7436	1.2607	0.0000	C	-2.3290	-1.0901	0.0000	H	-1.6935	2.7869	0.0000
C	4.7636	2.2586	0.0000	C	-4.7748	-0.6847	0.0000	H	0.9243	2.2405	0.0000
C	3.6365	-1.8239	0.0000	C	-5.8039	0.2024	0.0000	H	2.0467	-3.2479	0.0000
C	2.3398	-2.1913	0.0000	C	-5.5499	1.6064	0.0000	H	4.4372	-2.5727	0.0000
C	1.2842	-1.2080	0.0000	C	-4.2771	2.0806	0.0000	H	6.1377	-0.8558	0.0000
C	1.6138	0.1990	0.0000	C	-2.1389	-2.5474	0.0000	H	6.8026	1.5386	0.0000
C	-0.0460	-1.5650	0.0000	C	-0.8027	-2.8260	0.0000	H	5.0614	3.3123	0.0000
C	-1.0306	-0.5316	0.0000	H	-2.9604	-3.2613	0.0000	H	2.6511	2.6998	0.0000
C	-0.7449	0.8355	0.0000	H	-0.3354	-3.8089	0.0000				

Table 3.203: Table of thermodynamic data as a function of temperature for Benzo[*a*]cyclopenta[*fg*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.173	489.636	489.636	∞
100	99.328	337.634	726.885	-38.925	512.771	551.801	-288.225
200	194.534	434.044	556.411	-24.473	500.541	595.702	-155.578
250	250.264	483.392	536.848	-13.364	494.774	620.160	-129.573
298.15	304.709	532.138	532.138	0.000	489.636	644.788	-112.962
300	306.776	534.029	532.144	0.566	489.447	645.749	-112.433
350	361.122	585.442	536.080	17.277	484.711	672.185	-100.316
400	411.497	637.002	545.474	36.611	480.598	699.247	-91.310
450	457.107	688.151	558.491	58.347	477.035	726.796	-84.363
500	497.859	738.462	573.981	82.241	473.943	754.735	-78.845
600	566.171	835.519	609.556	135.578	468.905	811.392	-70.637
700	620.191	927.010	648.440	194.999	465.208	868.789	-64.828
800	663.529	1012.756	688.679	259.261	462.695	926.619	-60.501
900	698.867	1093.017	729.196	327.439	461.215	984.695	-57.149
1000	728.079	1168.209	769.378	398.831	460.627	1042.898	-54.474
1100	752.488	1238.781	808.876	472.895	460.762	1101.133	-52.287
1200	773.061	1305.163	847.495	549.201	461.498	1159.312	-50.462
1300	790.524	1367.749	885.131	627.404	462.678	1217.420	-48.916
1400	805.440	1426.893	921.735	707.221	464.187	1275.428	-47.586
1500	818.254	1482.911	957.296	788.422	465.956	1333.321	-46.429
1600	829.320	1536.081	991.823	870.814	467.871	1391.081	-45.413
1700	838.926	1586.654	1025.338	954.237	469.868	1448.698	-44.512
1800	847.303	1634.848	1057.871	1038.558	471.883	1506.253	-43.709
1900	854.643	1680.860	1089.458	1123.663	473.888	1563.650	-42.987
2000	861.101	1724.865	1120.137	1209.457	475.836	1620.966	-42.334
2100	866.809	1767.019	1149.944	1295.858	477.660	1678.174	-41.741
2200	871.873	1807.463	1178.918	1382.798	479.358	1735.301	-41.200
2300	876.383	1846.320	1207.097	1470.215	480.926	1792.353	-40.705
2400	880.414	1883.706	1234.515	1558.058	482.302	1849.298	-40.248
2500	884.030	1919.720	1261.207	1646.284	483.498	1906.289	-39.829
2600	887.284	1954.457	1287.206	1734.852	484.480	1963.134	-39.439
2700	890.221	1988.000	1312.544	1823.730	485.254	2020.008	-39.079
2800	892.881	2020.424	1337.250	1912.887	485.796	2076.877	-38.744
2900	895.295	2051.799	1361.351	2002.298	486.081	2133.684	-38.431
3000	897.494	2082.188	1384.875	2091.939	486.147	2190.509	-38.139
3100	899.501	2111.650	1407.847	2181.790	485.926	2247.268	-37.865
3200	901.337	2140.238	1430.290	2271.833	485.456	2304.103	-37.610
3300	903.021	2167.999	1452.226	2362.053	484.719	2360.992	-37.371
3400	904.570	2194.981	1473.677	2452.433	483.691	2417.830	-37.145
3500	905.996	2221.223	1494.662	2542.962	482.378	2474.687	-36.932
3600	907.312	2246.764	1515.201	2633.629	480.797	2531.662	-36.733
3700	908.530	2271.640	1535.310	2724.422	478.922	2588.701	-36.545
3800	909.658	2295.884	1555.008	2815.332	476.729	2645.741	-36.367
3900	910.705	2319.527	1574.309	2906.351	474.255	2702.797	-36.199
4000	911.679	2342.596	1593.229	2997.470	471.484	2760.043	-36.042
4100	912.586	2365.119	1611.782	3088.684	468.387	2817.296	-35.892
4200	913.431	2387.121	1629.981	3179.985	464.988	2874.621	-35.750
4300	914.222	2408.624	1647.840	3271.368	461.273	2931.951	-35.615
4400	914.961	2429.650	1665.371	3362.828	457.251	2989.452	-35.489
4500	915.653	2450.219	1682.584	3454.359	452.935	3047.098	-35.369
4600	916.303	2470.352	1699.491	3545.957	448.279	3104.850	-35.256
4700	916.913	2490.064	1716.103	3637.618	443.296	3162.606	-35.148
4800	917.487	2509.375	1732.429	3729.339	438.028	3220.566	-35.046
4900	918.027	2528.298	1748.479	3821.115	432.408	3278.518	-34.949
5000	918.536	2546.850	1764.261	3912.943	426.519	3336.754	-34.858

3.204. Naphth[1,2-*k*]acephenanthrylene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 201-27-4
Point Group: C_s

Length: 15.68 Å
Width: 9.114 Å
Breadth: 3.883 Å
L/B Ratio: 1.721

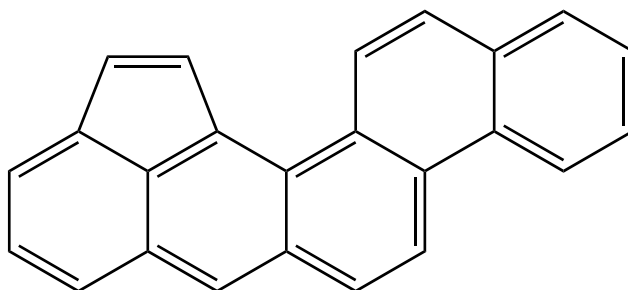
Cartesian coordinates:

C	-3.2290	0.1980	0.0000	C	-1.5208	1.8964	0.0000	H	4.4598	-2.7580	0.0000
C	-2.8368	1.5896	0.0000	C	-2.3622	-0.8781	0.0000	H	2.0407	-3.3142	0.0000
C	-4.1005	2.3468	0.0000	C	-5.2064	-1.1598	0.0000	H	1.1391	2.1763	0.0000
C	-5.1493	1.4787	0.0000	C	-4.3415	-2.2762	0.0000	H	-0.2954	-2.6066	0.0000
C	-4.6428	0.0955	0.0000	C	-2.9623	-2.1564	0.0000	H	-1.1599	2.9306	0.0000
C	3.6985	-1.9693	0.0000	C	3.1981	0.4416	0.0000	H	-6.2912	-1.3017	0.0000
C	2.3811	-2.2722	0.0000	C	4.1423	-0.5997	0.0000	H	-4.7876	-3.2769	0.0000
C	1.3830	-1.2341	0.0000	C	5.5179	-0.2929	0.0000	H	-2.3205	-3.0464	0.0000
C	1.7836	0.1220	0.0000	C	5.9378	1.0198	0.0000	H	6.2489	-1.1094	0.0000
C	0.8094	1.1242	0.0000	C	4.9976	2.0608	0.0000	H	7.0066	1.2576	0.0000
C	0.0221	-1.5541	0.0000	C	3.6494	1.7766	0.0000	H	5.3417	3.1002	0.0000
C	-0.9478	-0.5548	0.0000	H	-4.1453	3.4340	0.0000	H	2.8999	2.5829	0.0000
C	-0.5513	0.8150	0.0000	H	-6.2090	1.7263	0.0000				

Table 3.204: Table of thermodynamic data as a function of temperature for Naphth[1,2-*k*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.043	452.899	452.899	∞
100	98.776	339.240	726.952	-38.771	476.188	515.058	-269.033
200	193.676	435.070	557.093	-24.405	463.872	558.829	-145.948
250	249.568	484.244	537.581	-13.334	458.067	583.240	-121.859
298.15	304.165	532.880	532.880	0.000	452.899	607.830	-106.487
300	306.237	534.768	532.886	0.565	452.709	608.790	-105.997
350	360.708	586.108	536.816	17.252	447.949	635.190	-94.795
400	411.175	637.619	546.199	36.568	443.818	662.220	-86.475
450	456.852	688.734	559.202	58.289	440.240	689.739	-80.061
500	497.652	739.022	574.678	82.172	437.137	717.650	-74.971
600	566.031	836.047	610.226	135.492	432.082	774.253	-67.403
700	620.096	927.519	649.089	194.901	428.373	831.598	-62.053
800	663.468	1013.255	689.310	259.156	425.853	889.377	-58.069
900	698.832	1093.510	729.812	327.329	424.368	947.404	-54.985
1000	728.064	1168.700	769.981	398.719	423.778	1005.558	-52.524
1100	752.488	1239.271	809.470	472.782	423.912	1063.743	-50.512
1200	773.070	1305.654	848.080	549.088	424.648	1121.873	-48.833
1300	790.541	1368.241	885.708	627.292	425.829	1179.932	-47.409
1400	805.462	1427.386	922.307	707.112	427.341	1237.891	-46.185
1500	818.279	1483.406	957.863	788.315	429.112	1295.734	-45.121
1600	829.347	1536.578	992.385	870.709	431.029	1353.445	-44.185
1700	838.953	1587.152	1025.896	954.135	433.029	1411.012	-43.354
1800	847.331	1635.348	1058.426	1038.459	435.047	1468.518	-42.614
1900	854.670	1681.361	1090.010	1123.567	437.055	1525.864	-41.948
2000	861.129	1725.368	1120.686	1209.364	439.006	1583.130	-41.346
2100	866.835	1767.523	1150.491	1295.768	440.832	1640.288	-40.799
2200	871.899	1807.968	1179.464	1382.709	442.532	1697.364	-40.300
2300	876.408	1846.827	1207.640	1470.129	444.103	1754.366	-39.842
2400	880.438	1884.213	1235.057	1557.975	445.482	1811.260	-39.420
2500	884.053	1920.229	1261.748	1646.203	446.680	1868.200	-39.033
2600	887.305	1954.966	1287.746	1734.773	447.664	1924.994	-38.673
2700	890.242	1988.510	1313.082	1823.653	448.440	1981.817	-38.340
2800	892.900	2020.934	1337.787	1912.812	448.984	2038.636	-38.030
2900	895.314	2052.310	1361.888	2002.225	449.271	2095.392	-37.741
3000	897.512	2082.700	1385.411	2091.868	449.339	2152.165	-37.472
3100	899.518	2112.163	1408.382	2181.721	449.120	2208.873	-37.218
3200	901.354	2140.751	1430.824	2271.766	448.651	2265.656	-36.982
3300	903.037	2168.513	1452.760	2361.987	447.916	2322.494	-36.761
3400	904.585	2195.495	1474.210	2452.369	446.890	2379.281	-36.552
3500	906.010	2221.737	1495.195	2542.900	445.578	2436.086	-36.356
3600	907.326	2247.279	1515.733	2633.567	443.998	2493.010	-36.172
3700	908.543	2272.156	1535.842	2724.362	442.125	2549.997	-35.999
3800	909.671	2296.400	1555.539	2815.273	439.933	2606.985	-35.835
3900	910.717	2320.043	1574.840	2906.293	437.460	2663.990	-35.679
4000	911.690	2343.113	1593.759	2997.414	434.691	2721.184	-35.534
4100	912.597	2365.636	1612.312	3088.629	431.595	2778.386	-35.396
4200	913.442	2387.638	1630.511	3179.931	428.196	2835.659	-35.266
4300	914.232	2409.141	1648.370	3271.316	424.483	2892.937	-35.141
4400	914.971	2430.167	1665.900	3362.776	420.462	2950.387	-35.025
4500	915.663	2450.737	1683.113	3454.308	416.147	3007.981	-34.915
4600	916.312	2470.869	1700.020	3545.907	411.492	3065.682	-34.811
4700	916.922	2490.582	1716.631	3637.569	406.510	3123.386	-34.712
4800	917.495	2509.893	1732.957	3729.290	401.242	3181.293	-34.619
4900	918.035	2528.816	1749.007	3821.067	395.623	3239.194	-34.530
5000	918.544	2547.368	1764.789	3912.896	389.735	3297.378	-34.447

3.205. Indeno[7,1-*bc*]chrysene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 777080-23-6
Point Group: C₁

Length: 15.92 Å
Width: 9.190 Å
Breadth: 4.220 Å
L/B Ratio: 1.733

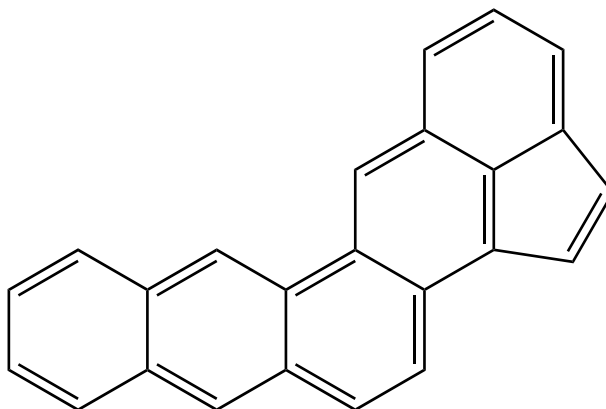
Cartesian coordinates:

C	1.8521	-2.2089	0.1360	C	5.2616	-0.9012	0.0532	H	4.9547	2.5315	-0.1287
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C	2.9534	-0.2041	0.0091	C	4.6619	1.4775	-0.0740	H	0.0585	3.5563	-0.0077
C	3.9428	-1.2428	0.0714	C	-1.2364	-1.6299	-0.1825	H	-2.3059	2.8368	0.0918
C	3.1829	-2.4958	0.1537	C	-2.5449	-2.0034	-0.1876	H	-2.8252	-3.0586	-0.2857
C	3.2695	1.1502	-0.0536	C	-3.5786	-1.0305	-0.0705	H	-0.4681	-2.4045	-0.2948
C	2.1769	2.0291	-0.0696	C	-3.2312	0.3297	0.0198	H	-4.0028	2.3530	0.1893
C	0.8717	1.5305	-0.0415	C	-4.9425	-1.4153	-0.0537	H	-6.3839	1.6448	0.2205
C	0.5589	0.1260	-0.0235	C	-5.9271	-0.4667	0.0500	H	-6.9823	-0.7583	0.0637
C	-0.2007	2.4906	-0.0065	C	-5.5866	0.8989	0.1386	H	-5.1946	-2.4794	-0.1259
C	-1.4910	2.0987	0.0412	C	-4.2720	1.2882	0.1225	H	3.6448	-3.4784	0.2237
C	-1.8430	0.7073	0.0078	H	6.0557	-1.6529	0.0973	H	1.0455	-2.9403	0.2021
C	-0.8416	-0.2639	-0.0577	H	6.6670	0.7460	-0.0414				

Table 3.205: Table of thermodynamic data as a function of temperature for Indeno[7,1-*bc*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-44.912	487.940	487.940	∞
100	98.030	337.658	724.551	-38.689	511.311	550.339	-287.462
200	193.325	433.108	554.984	-24.375	498.943	594.292	-155.210
250	249.278	482.211	535.494	-13.321	493.122	618.803	-129.289
298.15	303.878	530.798	530.798	0.000	487.940	643.492	-112.735
300	305.951	532.684	530.804	0.564	487.750	644.456	-112.207
350	360.414	583.979	534.730	17.237	482.975	670.962	-100.134
400	410.878	635.450	544.105	36.538	478.830	698.099	-91.161
450	456.557	686.530	557.098	58.245	475.237	725.728	-84.239
500	497.363	736.787	572.562	82.113	472.119	753.749	-78.742
600	565.744	833.760	608.086	135.404	467.036	810.578	-70.566
700	619.798	925.188	646.924	194.784	463.298	868.154	-64.781
800	663.155	1010.883	687.122	259.008	460.747	926.169	-60.471
900	698.503	1091.100	727.601	327.149	459.230	984.434	-57.134
1000	727.725	1166.254	767.749	398.505	458.606	1042.831	-54.471
1100	752.145	1236.793	807.216	472.534	458.706	1101.263	-52.294
1200	772.731	1303.146	845.807	548.807	459.408	1159.642	-50.477
1300	790.208	1365.706	883.416	626.977	460.556	1217.954	-48.937
1400	805.140	1424.828	919.996	706.764	462.034	1276.167	-47.613
1500	817.970	1480.825	955.535	787.935	463.774	1334.267	-46.462
1600	829.053	1533.978	990.041	870.300	465.661	1392.237	-45.451
1700	838.674	1584.534	1023.536	953.697	467.633	1450.065	-44.554
1800	847.066	1632.715	1056.051	1037.994	469.623	1507.833	-43.755
1900	854.420	1678.714	1087.622	1123.076	471.605	1565.444	-43.036
2000	860.893	1722.709	1118.284	1208.848	473.532	1622.975	-42.387
2100	866.613	1764.853	1148.077	1295.229	475.335	1680.399	-41.797
2200	871.689	1805.287	1177.037	1382.149	477.014	1737.743	-41.258
2300	876.210	1844.137	1205.203	1469.549	478.564	1795.013	-40.765
2400	880.251	1881.515	1232.609	1557.375	479.924	1852.177	-40.311
2500	883.877	1917.523	1259.289	1645.585	481.104	1909.387	-39.894
2600	887.139	1952.254	1285.278	1734.139	482.071	1966.452	-39.506
2700	890.085	1985.792	1310.605	1823.002	482.831	2023.547	-39.147
2800	892.752	2018.211	1335.301	1912.146	483.360	2080.637	-38.814
2900	895.174	2049.582	1359.394	2001.545	483.632	2137.666	-38.503
3000	897.379	2079.967	1382.909	2091.174	483.686	2194.712	-38.213
3100	899.392	2109.425	1405.872	2181.014	483.455	2251.693	-37.940
3200	901.234	2138.009	1428.307	2271.047	482.973	2308.751	-37.686
3300	902.923	2165.768	1450.236	2361.256	482.226	2365.863	-37.448
3400	904.476	2192.746	1471.680	2451.627	481.189	2422.925	-37.223
3500	905.907	2218.986	1492.658	2542.147	479.866	2480.005	-37.011
3600	907.228	2244.525	1513.190	2632.805	478.277	2537.204	-36.813
3700	908.449	2269.399	1533.294	2723.589	476.394	2594.467	-36.627
3800	909.581	2293.641	1552.985	2814.492	474.193	2651.731	-36.450
3900	910.632	2317.281	1572.281	2905.503	471.711	2709.011	-36.282
4000	911.609	2340.349	1591.195	2996.615	468.934	2766.482	-36.126
4100	912.519	2362.870	1609.743	3087.822	465.830	2823.960	-35.977
4200	913.367	2384.870	1627.937	3179.117	462.424	2881.510	-35.836
4300	914.160	2406.371	1645.791	3270.494	458.702	2939.065	-35.702
4400	914.902	2427.396	1663.317	3361.947	454.675	2996.792	-35.576
4500	915.597	2447.964	1680.526	3453.473	450.353	3054.663	-35.457
4600	916.249	2468.096	1697.429	3545.065	445.692	3112.641	-35.344
4700	916.861	2487.807	1714.037	3636.721	440.704	3170.623	-35.237
4800	917.437	2507.116	1730.359	3728.436	435.430	3228.807	-35.136
4900	917.979	2526.039	1746.405	3820.207	429.805	3286.986	-35.039
5000	918.490	2544.590	1762.183	3912.031	423.911	3345.448	-34.949

3.206. Cyclopenta[de]pentaphene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908069-18-1
Point Group: C_s

Length: 15.94 Å
Width: 9.192 Å
Breadth: 3.886 Å
L/B Ratio: 1.734

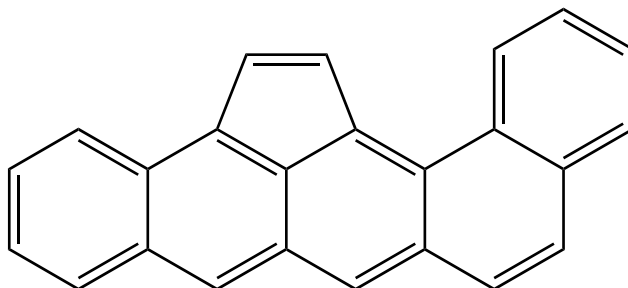
Cartesian coordinates:

C	-3.1030	-0.2356	0.0000	C	1.0705	0.2003	0.0000	H	6.2138	-2.5591	0.0000
C	-2.5689	1.0786	0.0000	C	1.6367	1.5091	0.0000	H	7.1868	-0.2820	0.0000
C	-3.7339	1.9796	0.0000	C	0.7668	2.6658	0.0000	H	5.7095	1.7191	0.0000
C	-4.8790	1.2401	0.0000	C	-0.5723	2.5314	0.0000	H	3.7473	-2.8753	0.0000
C	-4.5338	-0.1914	0.0000	C	-0.3831	0.0428	0.0000	H	3.4450	2.6818	0.0000
C	5.5398	-1.6961	0.0000	C	-1.1951	1.2286	0.0000	H	1.4841	-1.9125	0.0000
C	6.0973	-0.3915	0.0000	C	-0.9457	-1.2292	0.0000	H	1.2355	3.6570	0.0000
C	5.2877	0.7077	0.0000	C	-2.3480	-1.4013	0.0000	H	-1.2328	3.4067	0.0000
C	4.1858	-1.8711	0.0000	C	-5.2157	-1.3738	0.0000	H	-0.2909	-2.1146	0.0000
C	3.3146	-0.7425	0.0000	C	-4.4639	-2.5873	0.0000	H	-6.3092	-1.4132	0.0000
C	3.8700	0.5566	0.0000	C	-3.0917	-2.6195	0.0000	H	-5.0228	-3.5298	0.0000
C	3.0104	1.6743	0.0000	H	-3.6526	3.0651	0.0000	H	-2.5510	-3.5718	0.0000
C	1.9132	-0.8976	0.0000	H	-5.9022	1.6100	0.0000				

Table 3.206: Table of thermodynamic data as a function of temperature for Cyclopenta[de]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-45.210	480.471	480.471	∞
100	99.032	340.947	729.895	-38.895	503.636	542.335	-283.281
200	194.375	437.147	559.509	-24.472	491.377	585.918	-153.023
250	250.269	486.478	539.945	-13.367	485.606	610.221	-127.496
298.15	304.807	535.234	535.234	0.000	480.471	634.700	-111.195
300	306.877	537.126	535.239	0.566	480.282	635.656	-110.675
350	361.258	588.557	539.177	17.283	475.552	661.936	-98.787
400	411.633	640.136	548.575	36.624	471.447	688.842	-89.952
450	457.227	691.300	561.597	58.366	467.890	716.234	-83.137
500	497.960	741.623	577.092	82.266	464.803	744.015	-77.725
600	566.241	838.695	612.676	135.612	459.774	800.355	-69.676
700	620.245	930.195	651.569	195.039	456.083	857.434	-63.981
800	663.580	1015.948	691.816	259.306	453.575	914.945	-59.739
900	698.920	1096.215	732.339	327.489	452.100	972.701	-56.453
1000	728.134	1171.413	772.526	398.887	451.518	1030.585	-53.831
1100	752.546	1241.990	812.030	472.956	451.658	1088.499	-51.687
1200	773.120	1308.378	850.654	549.268	452.400	1146.356	-49.899
1300	790.584	1370.968	888.294	627.477	453.586	1204.143	-48.382
1400	805.500	1430.117	924.903	707.300	455.101	1261.829	-47.078
1500	818.312	1486.139	960.468	788.507	456.876	1319.399	-45.945
1600	829.377	1539.313	994.998	870.904	458.797	1376.836	-44.948
1700	838.980	1589.889	1028.516	954.333	460.800	1434.130	-44.065
1800	847.355	1638.086	1061.053	1038.659	462.820	1491.361	-43.277
1900	854.692	1684.101	1092.643	1123.770	464.830	1548.434	-42.569
2000	861.149	1728.109	1123.324	1209.568	466.783	1605.426	-41.929
2100	866.854	1770.265	1153.134	1295.974	468.611	1662.310	-41.347
2200	871.915	1810.710	1182.111	1382.918	470.313	1719.112	-40.816
2300	876.423	1849.570	1210.292	1470.339	471.885	1775.839	-40.330
2400	880.452	1886.957	1237.712	1558.187	473.266	1832.459	-39.882
2500	884.066	1922.973	1264.407	1646.416	474.465	1889.125	-39.470
2600	887.318	1957.711	1290.408	1734.988	475.451	1945.644	-39.088
2700	890.254	1991.255	1315.748	1823.869	476.228	2002.193	-38.734
2800	892.911	2023.680	1340.455	1913.029	476.773	2058.737	-38.405
2900	895.325	2055.056	1364.559	2002.443	477.061	2115.218	-38.098
3000	897.522	2085.447	1388.085	2092.087	477.130	2171.717	-37.812
3100	899.527	2114.910	1411.058	2181.941	476.912	2228.150	-37.543
3200	901.362	2143.498	1433.502	2271.987	476.444	2284.659	-37.292
3300	903.045	2171.260	1455.440	2362.208	475.709	2341.222	-37.058
3400	904.592	2198.242	1476.892	2452.591	474.684	2397.734	-36.836
3500	906.017	2224.485	1497.878	2543.123	473.373	2454.265	-36.627
3600	907.333	2250.027	1518.418	2633.791	471.794	2510.914	-36.432
3700	908.550	2274.904	1538.529	2724.586	469.921	2567.626	-36.248
3800	909.677	2299.148	1558.228	2815.498	467.730	2624.339	-36.073
3900	910.723	2322.791	1577.530	2906.519	465.258	2681.069	-35.908
4000	911.696	2345.861	1596.451	2997.640	462.489	2737.988	-35.754
4100	912.602	2368.385	1615.005	3088.856	459.394	2794.915	-35.607
4200	913.447	2390.386	1633.206	3180.158	455.996	2851.914	-35.468
4300	914.237	2411.890	1651.066	3271.543	452.282	2908.917	-35.336
4400	914.975	2432.916	1668.597	3363.004	448.262	2966.092	-35.211
4500	915.667	2453.486	1685.811	3454.537	443.948	3023.411	-35.094
4600	916.316	2473.619	1702.719	3546.136	439.293	3080.837	-34.983
4700	916.926	2493.332	1719.332	3637.799	434.312	3138.266	-34.877
4800	917.499	2512.642	1735.659	3729.520	429.044	3195.898	-34.778
4900	918.039	2531.566	1751.709	3821.297	423.426	3253.524	-34.682
5000	918.548	2550.118	1767.493	3913.127	417.538	3311.434	-34.594

3.207. Benzo[*a*]cyclopenta[*op*]naphthacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908069-25-0
Point Group: C_s

Length: 15.95 Å
Width: 9.173 Å
Breadth: 3.907 Å
L/B Ratio: 1.739

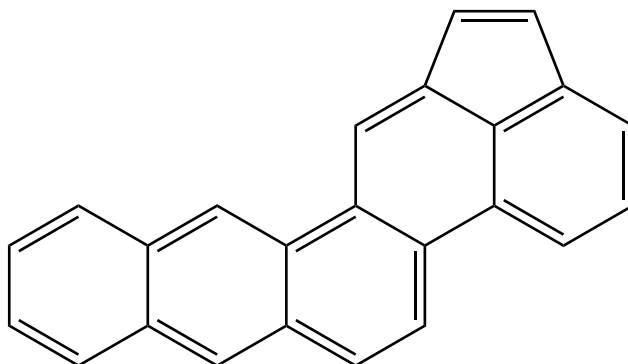
Cartesian coordinates:

C	-0.4061	-0.6590	-0.0040	C	4.3367	-1.5416	-0.0038	H	5.0895	2.2915	0.0105
C	-1.5241	0.1569	-0.0002	C	-2.4079	2.4992	-0.0049	H	4.1101	-2.6140	-0.0077
C	-1.2832	1.5872	0.0002	C	-3.6766	2.0546	-0.0096	H	2.7207	2.8071	0.0097
C	-0.0185	2.1488	0.0031	C	-3.9607	0.6402	-0.0050	H	0.1074	3.2387	0.0042
C	1.1364	1.3264	0.0034	C	-2.9116	-0.3012	0.0027	H	-2.1930	3.5749	-0.0060
C	0.8916	-0.0482	-0.0013	C	-5.3018	0.2197	-0.0057	H	-4.5229	2.7515	-0.0155
C	1.9111	-1.0282	-0.0043	C	-5.6145	-1.1248	0.0033	H	-6.1003	0.9708	-0.0131
C	3.2398	-0.6206	-0.0015	C	-4.5852	-2.0686	0.0148	H	-6.6591	-1.4523	0.0024
C	3.5083	0.7892	0.0038	C	-3.2641	-1.6626	0.0150	H	-4.8284	-3.1363	0.0239
C	2.4812	1.7371	0.0060	C	1.2230	-2.3213	-0.0110	H	-2.4872	-2.4358	0.0263
C	4.8806	1.2154	0.0066	C	-0.1230	-2.1075	-0.0113	H	1.7369	-3.2808	-0.0156
C	5.8933	0.3102	0.0043	H	6.4602	-1.7897	-0.0025	H	-0.8835	-2.8886	-0.0178
C	5.6182	-1.0899	-0.0009	H	6.9380	0.6381	0.0064				

Table 3.207: Table of thermodynamic data as a function of temperature for Benzo[*a*]cyclopenta[*op*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.202	499.641	499.641	∞
100	99.181	337.994	727.374	-38.938	522.763	561.757	-293.426
200	194.617	434.355	556.814	-24.492	510.527	605.627	-158.170
250	250.459	483.734	537.236	-13.376	504.767	630.068	-131.643
298.15	304.985	532.521	532.521	0.000	499.641	654.679	-114.695
300	307.055	534.414	532.527	0.566	499.452	655.639	-114.155
350	361.465	585.875	536.467	17.293	494.732	682.055	-101.789
400	411.882	637.484	545.870	36.645	490.637	709.094	-92.596
450	457.514	688.679	558.900	58.401	487.094	736.617	-85.503
500	498.270	739.034	574.404	82.315	484.022	764.529	-79.868
600	566.555	836.164	610.009	135.693	479.025	821.125	-71.484
700	620.523	927.710	648.925	195.150	475.364	878.454	-65.550
800	663.805	1013.497	689.194	259.442	472.881	936.212	-61.127
900	699.090	1093.787	729.737	327.645	471.426	994.212	-57.701
1000	728.256	1169.000	769.943	399.057	470.858	1052.338	-54.967
1100	752.628	1239.587	809.463	473.137	471.009	1110.492	-52.732
1200	773.170	1305.980	848.101	549.455	471.757	1168.590	-50.866
1300	790.610	1368.574	885.753	627.668	472.947	1226.616	-49.285
1400	805.507	1427.724	922.372	707.493	474.464	1284.541	-47.926
1500	818.307	1483.746	957.946	788.699	476.238	1342.350	-46.744
1600	829.361	1536.920	992.485	871.096	478.158	1400.027	-45.705
1700	838.958	1587.494	1026.010	954.523	480.159	1457.560	-44.784
1800	847.328	1635.690	1058.553	1038.847	482.177	1515.031	-43.964
1900	854.662	1681.703	1090.148	1123.954	484.184	1572.344	-43.226
2000	861.116	1725.709	1120.834	1209.750	486.134	1629.575	-42.559
2100	866.820	1767.864	1150.649	1296.152	487.958	1686.699	-41.953
2200	871.882	1808.308	1179.629	1383.092	489.657	1743.742	-41.401
2300	876.389	1847.166	1207.813	1470.510	491.226	1800.709	-40.895
2400	880.419	1884.551	1235.237	1558.354	492.603	1857.569	-40.428
2500	884.033	1920.566	1261.934	1646.580	493.799	1914.476	-40.000
2600	887.286	1955.303	1287.938	1735.149	494.782	1971.236	-39.602
2700	890.222	1988.846	1313.280	1824.027	495.556	2028.026	-39.234
2800	892.881	2021.270	1337.990	1913.184	496.098	2084.810	-38.892
2900	895.295	2052.645	1362.095	2002.595	496.383	2141.533	-38.572
3000	897.493	2083.034	1385.622	2092.236	496.449	2198.273	-38.275
3100	899.500	2112.496	1408.597	2182.087	496.228	2254.947	-37.995
3200	901.336	2141.084	1431.043	2272.130	495.757	2311.698	-37.734
3300	903.020	2168.845	1452.982	2362.349	495.020	2368.502	-37.489
3400	904.568	2195.826	1474.435	2452.730	493.993	2425.256	-37.259
3500	905.994	2222.068	1495.423	2543.259	492.679	2482.028	-37.041
3600	907.310	2247.610	1515.964	2633.925	491.098	2538.919	-36.838
3700	908.528	2272.486	1536.076	2724.717	489.222	2595.873	-36.646
3800	909.656	2296.730	1555.775	2815.627	487.029	2652.828	-36.465
3900	910.703	2320.372	1575.079	2906.646	484.555	2709.799	-36.293
4000	911.676	2343.442	1594.001	2997.765	481.784	2766.961	-36.132
4100	912.583	2365.965	1612.555	3088.979	478.687	2824.129	-35.979
4200	913.429	2387.966	1630.757	3180.280	475.287	2881.370	-35.834
4300	914.219	2409.469	1648.617	3271.663	471.572	2938.615	-35.696
4400	914.958	2430.495	1666.149	3363.122	467.550	2996.032	-35.567
4500	915.651	2451.065	1683.364	3454.653	463.234	3053.594	-35.444
4600	916.301	2471.197	1700.273	3546.251	458.578	3111.261	-35.329
4700	916.911	2490.909	1716.886	3637.912	453.595	3168.933	-35.218
4800	917.485	2510.220	1733.213	3729.632	448.326	3226.807	-35.114
4900	918.025	2529.143	1749.264	3821.408	442.706	3284.675	-35.014
5000	918.534	2547.695	1765.048	3913.236	436.817	3342.827	-34.922

3.208. Benzo[*b*]cyclopenta[*hi*]chrysene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908069-32-9
Point Group: C_s

Length: 15.94 Å
Width: 9.160 Å
Breadth: 3.887 Å
L/B Ratio: 1.740

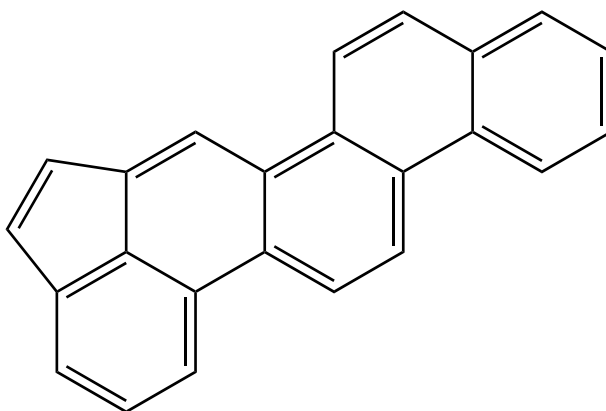
Cartesian coordinates:

C	-5.4009	0.1576	0.0000	C	1.0755	0.1162	0.0000	H	6.3164	-2.4604	0.0000
C	-4.4505	-0.8296	0.0000	C	2.9697	1.6549	0.0000	H	7.2077	-0.1512	0.0000
C	-3.0798	-0.4429	0.0000	C	3.8609	0.5730	0.0000	H	5.6621	1.7975	0.0000
C	-2.6278	0.8638	0.0000	C	3.3502	-0.7490	0.0000	H	3.8631	-2.8660	0.0000
C	-3.6333	1.8662	0.0000	C	1.9639	-0.9557	0.0000	H	3.3646	2.6786	0.0000
C	-4.9641	1.5094	0.0000	C	5.2772	0.7715	0.0000	H	1.5694	-1.9844	0.0000
C	-1.2012	1.0366	0.0000	C	6.1225	-0.2964	0.0000	H	1.1093	3.5706	0.0000
C	-0.3624	-0.0844	0.0000	C	5.6101	-1.6237	0.0000	H	-1.3628	3.1993	0.0000
C	-0.8893	-1.4224	0.0000	C	4.2665	-1.8472	0.0000	H	-0.1867	-2.2688	0.0000
C	-2.2379	-1.6021	0.0000	C	-3.1588	-2.7522	0.0000	H	-3.3176	2.9186	0.0000
C	-0.6506	2.3609	0.0000	C	-4.4449	-2.3030	0.0000	H	-5.7279	2.2949	0.0000
C	0.6873	2.5590	0.0000	H	-2.8231	-3.7872	0.0000	H	-6.4709	-0.0709	0.0000
C	1.5944	1.4422	0.0000	H	-5.3518	-2.9043	0.0000				

Table 3.208: Table of thermodynamic data as a function of temperature for Benzo[*b*]cyclopenta[*hi*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.320	470.677	470.677	∞
100	99.579	341.674	731.345	-38.967	493.770	532.396	-278.090
200	194.701	438.171	560.687	-24.503	481.552	575.888	-150.403
250	250.575	487.572	541.100	-13.382	475.797	600.138	-125.389
298.15	305.131	536.383	536.383	0.000	470.677	624.563	-109.419
300	307.202	538.277	536.389	0.566	470.489	625.517	-108.910
350	361.612	589.761	540.330	17.301	465.776	651.739	-97.265
400	412.007	641.388	549.737	36.660	461.688	678.583	-88.612
450	457.610	692.596	562.772	58.421	458.150	705.911	-81.938
500	498.339	742.960	578.281	82.340	455.083	733.626	-76.640
600	566.589	840.099	613.895	135.722	450.090	789.830	-68.759
700	620.547	931.649	652.818	195.182	446.432	846.765	-63.185
800	663.834	1017.439	693.093	259.477	443.952	904.129	-59.032
900	699.130	1097.734	733.642	327.683	442.500	961.735	-55.816
1000	728.307	1172.952	773.852	399.100	441.937	1019.465	-53.250
1100	752.689	1243.544	813.376	473.185	442.093	1077.224	-51.152
1200	773.239	1309.943	852.018	549.510	442.848	1134.926	-49.401
1300	790.682	1372.542	889.673	627.729	444.044	1192.556	-47.916
1400	805.582	1431.698	926.296	707.562	445.569	1250.084	-46.640
1500	818.382	1487.724	961.874	788.776	447.351	1307.495	-45.530
1600	829.436	1540.903	996.416	871.180	449.278	1364.774	-44.554
1700	839.031	1591.482	1029.944	954.614	451.287	1421.909	-43.689
1800	847.399	1639.682	1062.490	1038.945	453.311	1478.981	-42.918
1900	854.731	1685.699	1094.089	1124.060	455.326	1535.894	-42.224
2000	861.182	1729.708	1124.777	1209.862	457.282	1592.725	-41.597
2100	866.884	1771.866	1154.594	1296.271	459.113	1649.449	-41.027
2200	871.942	1812.313	1183.578	1383.217	460.819	1706.091	-40.507
2300	876.447	1851.174	1211.764	1470.641	462.393	1762.658	-40.030
2400	880.473	1888.561	1239.190	1558.491	463.776	1819.117	-39.591
2500	884.085	1924.579	1265.890	1646.722	464.977	1875.623	-39.188
2600	887.335	1959.318	1291.896	1735.296	465.965	1931.981	-38.813
2700	890.269	1992.862	1317.240	1824.178	466.744	1988.370	-38.467
2800	892.926	2025.288	1341.952	1913.340	467.290	2044.753	-38.145
2900	895.338	2056.664	1366.059	2002.755	467.580	2101.073	-37.844
3000	897.534	2087.055	1389.588	2092.401	467.650	2157.411	-37.563
3100	899.538	2116.518	1412.565	2182.256	467.433	2213.684	-37.300
3200	901.372	2145.107	1435.012	2272.303	466.966	2270.032	-37.054
3300	903.055	2172.870	1456.953	2362.525	466.232	2326.433	-36.824
3400	904.601	2199.852	1478.408	2452.909	465.208	2382.785	-36.606
3500	906.026	2226.095	1499.397	2543.441	463.897	2439.154	-36.402
3600	907.341	2251.637	1519.940	2634.110	462.320	2495.643	-36.210
3700	908.557	2276.514	1540.053	2724.906	460.447	2552.194	-36.030
3800	909.683	2300.759	1559.754	2815.819	458.257	2608.746	-35.859
3900	910.729	2324.402	1579.058	2906.840	455.785	2665.315	-35.697
4000	911.702	2347.472	1597.982	2997.962	453.017	2722.073	-35.546
4100	912.608	2369.996	1616.538	3089.178	449.922	2778.839	-35.402
4200	913.453	2391.998	1634.740	3180.482	446.525	2835.676	-35.266
4300	914.242	2413.501	1652.602	3271.867	442.812	2892.518	-35.136
4400	914.980	2434.527	1670.135	3363.328	438.793	2949.532	-35.015
4500	915.672	2455.097	1687.350	3454.861	434.479	3006.690	-34.900
4600	916.321	2475.230	1704.260	3546.461	429.825	3063.954	-34.792
4700	916.930	2494.943	1720.874	3638.124	424.843	3121.223	-34.688
4800	917.503	2514.254	1737.203	3729.846	419.576	3178.694	-34.591
4900	918.043	2533.178	1753.254	3821.624	413.958	3236.158	-34.497
5000	918.551	2551.730	1769.039	3913.454	408.071	3293.907	-34.410

3.209. Cyclopenta[de]picene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908069-39-6
Point Group: C_s

Length: 15.88 Å
Width: 9.017 Å
Breadth: 3.883 Å
L/B Ratio: 1.761

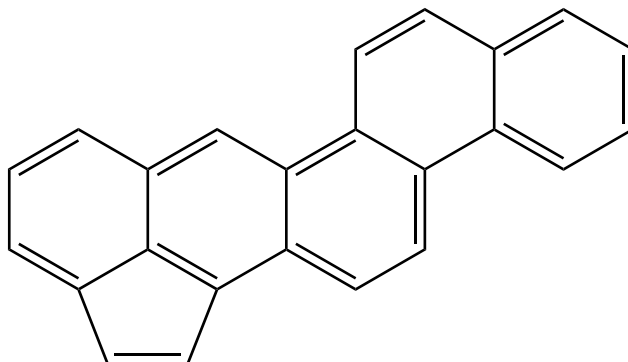
Cartesian coordinates:

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C	0.4228	-0.4754	0.0000	C	-5.2178	-1.1746	0.0000	H	-3.3740	-3.1301	0.0000
C	0.9481	0.8313	0.0000	C	2.3768	1.0319	0.0000	H	-0.9161	-2.8241	0.0000
C	0.0775	1.9510	0.0000	C	5.2365	1.0643	0.0000	H	-3.7307	2.4204	0.0000
C	-1.2756	1.7790	0.0000	C	4.4682	2.2556	0.0000	H	-6.1978	2.0765	0.0000
C	-1.0022	-0.6456	0.0000	C	3.0879	2.2572	0.0000	H	-7.1413	-0.2195	0.0000
C	-1.8424	0.4758	0.0000	C	3.8202	-2.3270	0.0000	H	-5.6261	-2.1916	0.0000
C	-2.9348	-2.1258	0.0000	C	4.9458	-1.5601	0.0000	H	6.3293	1.1164	0.0000
C	-1.5898	-1.9540	0.0000	C	4.5700	-0.1354	0.0000	H	5.0022	3.2122	0.0000
C	-3.8153	-0.9967	0.0000	C	3.1488	-0.1135	0.0000	H	2.5156	3.1946	0.0000
C	-3.2760	0.3017	0.0000	C	2.6325	-1.4548	0.0000	H	3.7636	-3.4136	0.0000
C	-4.1590	1.4065	0.0000	H	0.8338	-2.6342	0.0000	H	5.9777	-1.9054	0.0000
C	-5.5199	1.2167	0.0000	H	0.5292	2.9534	0.0000				

Table 3.209: Table of thermodynamic data as a function of temperature for Cyclopenta[de]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-45.246	459.424	459.424	∞
100	99.825	341.020	729.869	-38.885	482.599	521.291	-272.289
200	194.219	437.434	559.620	-24.437	470.365	564.848	-147.520
250	249.886	486.703	540.085	-13.346	464.580	589.139	-123.091
298.15	304.322	535.381	535.381	0.000	459.424	613.609	-107.500
300	306.389	537.270	535.387	0.565	459.234	614.564	-107.003
350	360.747	588.624	539.319	17.257	454.479	640.840	-95.638
400	411.141	640.135	548.703	36.573	450.348	667.743	-87.197
450	456.769	691.243	561.707	58.291	446.767	695.137	-80.688
500	497.536	741.520	577.183	82.169	443.659	722.922	-75.522
600	565.865	838.520	612.728	135.475	438.590	779.277	-67.841
700	619.891	929.964	651.585	194.865	434.862	836.376	-62.410
800	663.231	1015.670	691.797	259.098	432.320	893.912	-58.365
900	698.571	1095.896	732.289	327.246	430.810	951.699	-55.234
1000	727.787	1171.057	772.448	398.609	430.193	1009.616	-52.736
1100	752.204	1241.601	811.925	472.644	430.299	1067.567	-50.693
1200	772.787	1307.959	850.524	548.922	431.007	1125.465	-48.989
1300	790.262	1370.524	888.141	627.098	432.160	1183.295	-47.544
1400	805.191	1429.649	924.728	706.889	433.643	1241.026	-46.302
1500	818.019	1485.650	960.273	788.066	435.388	1298.644	-45.222
1600	829.099	1538.806	994.784	870.435	437.280	1356.131	-44.272
1700	838.717	1589.365	1028.284	953.837	439.256	1413.477	-43.430
1800	847.107	1637.548	1060.805	1038.137	441.250	1470.761	-42.680
1900	854.459	1683.550	1092.379	1123.224	443.237	1527.889	-42.004
2000	860.929	1727.546	1123.046	1209.000	445.167	1584.936	-41.393
2100	866.648	1769.692	1152.842	1295.385	446.974	1641.876	-40.839
2200	871.721	1810.127	1181.806	1382.308	448.656	1698.737	-40.332
2300	876.241	1848.979	1209.974	1469.710	450.209	1755.522	-39.868
2400	880.280	1886.358	1237.383	1557.540	451.572	1812.202	-39.441
2500	883.904	1922.368	1264.067	1645.753	452.755	1868.928	-39.048
2600	887.165	1957.100	1290.058	1734.309	453.725	1925.508	-38.683
2700	890.109	1990.638	1315.388	1823.175	454.487	1982.118	-38.346
2800	892.775	2023.058	1340.086	1912.321	455.018	2038.724	-38.032
2900	895.196	2054.429	1364.180	2001.722	455.293	2095.268	-37.739
3000	897.400	2084.816	1387.698	2091.353	455.349	2151.830	-37.466
3100	899.412	2114.274	1410.663	2181.195	455.119	2208.326	-37.209
3200	901.253	2142.859	1433.100	2271.230	454.640	2264.899	-36.970
3300	902.941	2170.618	1455.030	2361.441	453.895	2321.525	-36.746
3400	904.493	2197.597	1476.476	2451.814	452.860	2378.102	-36.534
3500	905.923	2223.837	1497.456	2542.335	451.538	2434.697	-36.335
3600	907.243	2249.377	1517.989	2632.995	449.951	2491.411	-36.149
3700	908.464	2274.251	1538.094	2723.781	448.069	2548.189	-35.973
3800	909.595	2298.493	1557.787	2814.684	445.869	2604.968	-35.807
3900	910.645	2322.134	1577.084	2905.697	443.389	2661.763	-35.650
4000	911.621	2345.202	1595.999	2996.811	440.613	2718.748	-35.502
4100	912.531	2367.724	1614.548	3088.019	437.510	2775.741	-35.363
4200	913.379	2389.724	1632.744	3179.315	434.105	2832.805	-35.230
4300	914.171	2411.226	1650.599	3270.693	430.385	2889.875	-35.104
4400	914.913	2432.250	1668.126	3362.148	426.359	2947.117	-34.986
4500	915.607	2452.819	1685.336	3453.674	422.038	3004.502	-34.875
4600	916.258	2472.950	1702.240	3545.268	417.378	3061.995	-34.769
4700	916.870	2492.662	1718.848	3636.924	412.390	3119.491	-34.669
4800	917.446	2511.971	1735.171	3728.641	407.118	3177.190	-34.574
4900	917.988	2530.894	1751.218	3820.412	401.493	3234.883	-34.484
5000	918.498	2549.445	1766.998	3912.237	395.601	3292.860	-34.400

3.210. Indeno[1,7-*ab*]chrysene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 148292-86-8
Point Group: C_s

Length: 16.08 Å
Width: 9.081 Å
Breadth: 3.884 Å
L/B Ratio: 1.771

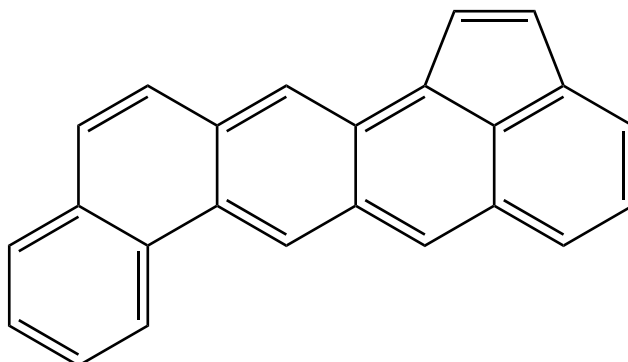
Cartesian coordinates:

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C	-3.8026	-0.9897	0.0000	C	2.2889	1.2091	0.0000	H	6.5346	-0.2525	0.0000
C	-3.3007	0.3253	0.0000	C	3.1326	0.0778	0.0000	H	3.4457	-3.2929	0.0000
C	-4.2205	1.4044	0.0000	C	2.6953	-1.2441	0.0000	H	0.8970	-2.4582	0.0000
C	-5.5722	1.1738	0.0000	C	1.3034	-1.4351	0.0000	H	0.3899	3.1180	0.0000
C	-6.0696	-0.1456	0.0000	C	3.7282	-2.2348	0.0000	H	-2.0662	2.7090	0.0000
C	-1.8783	0.5387	0.0000	C	5.0446	-1.8563	0.0000	H	-3.2982	-3.1068	0.0000
C	-1.0100	-0.5510	0.0000	C	5.4662	-0.4886	0.0000	H	-0.8489	-2.7213	0.0000
C	-1.5499	-1.8728	0.0000	C	4.5098	0.4816	0.0000	H	-3.8236	2.4308	0.0000
C	-2.8929	-2.0885	0.0000	C	4.4809	1.9538	0.0000	H	-6.2769	2.0118	0.0000
C	-1.3483	1.8743	0.0000	C	3.1848	2.3774	0.0000	H	-7.1519	-0.3106	0.0000
C	-0.0152	2.0993	0.0000	H	5.3763	2.5716	0.0000	H	-5.5793	-2.2375	0.0000
C	0.9146	1.0063	0.0000	H	2.8290	3.4061	0.0000				

Table 3.210: Table of thermodynamic data as a function of temperature for Indeno[1,7-*ab*]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-45.426	478.697	478.697	∞
100	100.101	342.096	732.448	-39.035	501.721	540.306	-282.221
200	195.041	438.873	561.532	-24.532	489.543	583.739	-152.454
250	250.869	488.345	541.924	-13.395	483.804	607.952	-127.022
298.15	305.365	537.203	537.203	0.000	478.697	632.338	-110.781
300	307.433	539.098	537.209	0.567	478.508	633.290	-110.263
350	361.787	590.613	541.153	17.311	473.806	659.470	-98.419
400	412.141	642.261	550.565	36.678	469.726	686.271	-89.616
450	457.713	693.484	563.606	58.445	466.194	713.555	-82.826
500	498.417	743.857	579.120	82.368	463.131	741.226	-77.434
600	566.626	841.006	614.745	135.756	458.144	797.339	-69.413
700	620.547	932.559	653.677	195.218	454.487	854.184	-63.739
800	663.800	1018.347	693.958	259.511	452.006	911.456	-59.511
900	699.069	1098.636	734.511	327.712	450.549	968.972	-56.236
1000	728.227	1173.846	774.724	399.122	449.979	1026.612	-53.624
1100	752.594	1244.430	814.250	473.199	450.126	1084.282	-51.487
1200	773.135	1310.820	852.892	549.514	450.871	1141.896	-49.704
1300	790.574	1373.411	890.548	627.722	452.057	1199.438	-48.193
1400	805.473	1432.559	927.170	707.544	453.570	1256.880	-46.894
1500	818.273	1488.578	962.747	788.747	455.342	1314.206	-45.764
1600	829.330	1541.750	997.287	871.140	457.258	1371.399	-44.771
1700	838.928	1592.322	1030.814	954.564	459.256	1428.450	-43.890
1800	847.300	1640.516	1063.358	1038.885	461.271	1485.438	-43.105
1900	854.636	1686.528	1094.955	1123.990	463.276	1542.268	-42.399
2000	861.092	1730.533	1125.641	1209.783	465.223	1599.017	-41.761
2100	866.798	1772.687	1155.457	1296.183	467.045	1655.658	-41.181
2200	871.860	1813.129	1184.438	1383.121	468.742	1712.219	-40.652
2300	876.369	1851.986	1212.622	1470.537	470.309	1768.704	-40.168
2400	880.400	1889.371	1240.046	1558.379	471.684	1825.082	-39.721
2500	884.015	1925.385	1266.744	1646.603	472.878	1881.507	-39.311
2600	887.269	1960.122	1292.748	1735.170	473.859	1937.785	-38.930
2700	890.206	1993.663	1318.091	1824.046	474.631	1994.093	-38.577
2800	892.866	2026.087	1342.800	1913.202	475.172	2050.396	-38.250
2900	895.281	2057.462	1366.906	2002.611	475.455	2106.637	-37.944
3000	897.480	2087.851	1390.434	2092.251	475.520	2162.895	-37.659
3100	899.487	2117.312	1413.409	2182.101	475.298	2219.088	-37.391
3200	901.324	2145.899	1435.854	2272.143	474.826	2275.357	-37.141
3300	903.009	2173.660	1457.794	2362.361	474.087	2331.679	-36.907
3400	904.557	2200.641	1479.247	2452.740	473.059	2387.952	-36.686
3500	905.984	2226.883	1500.235	2543.268	471.744	2444.242	-36.478
3600	907.301	2252.424	1520.776	2633.933	470.162	2500.652	-36.283
3700	908.519	2277.300	1540.888	2724.725	468.286	2557.124	-36.099
3800	909.647	2301.544	1560.587	2815.634	466.092	2613.598	-35.926
3900	910.695	2325.186	1579.891	2906.652	463.616	2670.088	-35.761
4000	911.669	2348.255	1598.813	2997.770	460.845	2726.768	-35.607
4100	912.576	2370.778	1617.367	3088.983	457.747	2783.456	-35.461
4200	913.422	2392.779	1635.569	3180.284	454.346	2840.215	-35.323
4300	914.212	2414.282	1653.429	3271.666	450.630	2896.979	-35.191
4400	914.952	2435.308	1670.961	3363.124	446.608	2953.915	-35.067
4500	915.645	2455.877	1688.176	3454.654	442.291	3010.995	-34.950
4600	916.295	2476.009	1705.085	3546.252	437.634	3068.181	-34.840
4700	916.905	2495.722	1721.698	3637.912	432.651	3125.371	-34.734
4800	917.479	2515.032	1738.025	3729.632	427.381	3182.765	-34.635
4900	918.020	2533.955	1754.076	3821.407	421.760	3240.152	-34.540
5000	918.529	2552.507	1769.860	3913.234	415.871	3297.822	-34.451

3.211. Benzo[*a*]cyclopenta[*hi*]naphthacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 908069-47-6
Point Group: C_s

Length: 16.00 Å
Width: 8.999 Å
Breadth: 3.884 Å
L/B Ratio: 1.778

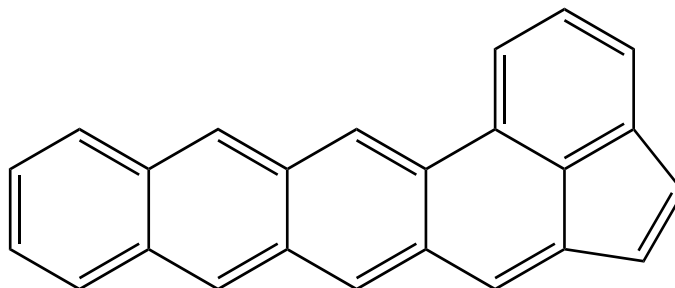
Cartesian coordinates:

C	3.6278	1.7614	0.0000	C	0.8195	1.0213	0.0000	H	-6.1411	2.4548	0.0000
C	3.2173	0.4174	0.0000	C	-2.2729	-1.0387	0.0000	H	-6.6274	0.0278	0.0000
C	4.1917	-0.5951	0.0000	C	-3.2041	0.0076	0.0000	H	-3.8345	3.3421	0.0000
C	5.5540	-0.2509	0.0000	C	-2.8905	1.3726	0.0000	H	-1.2212	2.7473	0.0000
C	5.9379	1.0766	0.0000	C	-1.5357	1.6970	0.0000	H	-0.1721	-2.7516	0.0000
C	4.9704	2.0868	0.0000	C	-4.0188	2.2624	0.0000	H	1.1084	2.0853	0.0000
C	3.7886	-1.9830	0.0000	C	-5.2901	1.7644	0.0000	H	2.1811	-3.3822	0.0000
C	2.4863	-2.3292	0.0000	C	-5.5843	0.3584	0.0000	H	4.5770	-2.7446	0.0000
C	1.4431	-1.3268	0.0000	C	-4.5461	-0.5182	0.0000	H	6.3097	-1.0447	0.0000
C	1.8049	0.0602	0.0000	C	-4.3851	-1.9813	0.0000	H	7.0000	1.3424	0.0000
C	0.1156	-1.6927	0.0000	C	-3.0549	-2.2841	0.0000	H	5.2811	3.1366	0.0000
C	-0.9088	-0.7138	0.0000	H	-5.2205	-2.6780	0.0000	H	2.8568	2.5472	0.0000
C	-0.5590	0.6760	0.0000	H	-2.6053	-3.2753	0.0000				

Table 3.211: Table of thermodynamic data as a function of temperature for Benzo[*a*]cyclopenta[*hi*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.042	488.074	488.074	∞
100	98.443	337.976	726.092	-38.812	511.322	550.318	-287.451
200	193.936	433.758	556.001	-24.448	499.003	594.222	-155.192
250	250.035	483.014	536.452	-13.360	493.216	618.697	-129.267
298.15	304.731	531.743	531.743	0.000	488.074	643.343	-112.709
300	306.806	533.634	531.748	0.566	487.884	644.306	-112.181
350	361.308	585.064	535.686	17.283	483.154	670.761	-100.103
400	411.767	636.655	545.084	36.629	479.053	697.841	-91.127
450	457.418	687.839	558.108	58.379	475.504	725.406	-84.201
500	498.186	738.184	573.607	82.289	472.428	753.360	-78.701
600	566.495	835.300	609.202	135.659	467.424	810.042	-70.519
700	620.497	926.840	648.109	195.111	463.758	867.458	-64.729
800	663.816	1012.626	688.371	259.403	461.275	925.303	-60.415
900	699.136	1092.919	728.909	327.609	459.823	983.390	-57.073
1000	728.330	1168.139	769.112	399.027	459.261	1041.602	-54.407
1100	752.723	1238.734	808.629	473.115	459.420	1099.842	-52.226
1200	773.280	1305.136	847.266	549.444	460.179	1158.025	-50.406
1300	790.728	1367.739	884.917	627.668	461.379	1216.135	-48.864
1400	805.630	1426.898	921.537	707.505	462.909	1274.143	-47.538
1500	818.430	1482.928	957.112	788.724	464.695	1332.035	-46.385
1600	829.484	1536.109	991.651	871.133	466.627	1389.793	-45.371
1700	839.078	1586.691	1025.178	954.572	468.641	1447.407	-44.472
1800	847.444	1634.894	1057.723	1038.907	470.670	1504.958	-43.672
1900	854.774	1680.913	1089.321	1124.026	472.689	1562.350	-42.951
2000	861.224	1724.925	1120.009	1209.833	474.650	1619.660	-42.300
2100	866.923	1767.085	1149.825	1296.246	476.485	1676.862	-41.709
2200	871.979	1807.533	1178.808	1383.196	478.194	1733.982	-41.169
2300	876.482	1846.395	1206.994	1470.623	479.772	1791.026	-40.675
2400	880.507	1883.785	1234.420	1558.477	481.158	1847.963	-40.219
2500	884.117	1919.803	1261.119	1646.711	482.363	1904.947	-39.801
2600	887.366	1954.544	1287.125	1735.288	483.354	1961.783	-39.412
2700	890.298	1988.089	1312.469	1824.174	484.135	2018.648	-39.052
2800	892.953	2020.516	1337.181	1913.338	484.685	2075.509	-38.718
2900	895.364	2051.893	1361.288	2002.756	484.977	2132.306	-38.406
3000	897.559	2082.285	1384.817	2092.404	485.050	2189.121	-38.115
3100	899.562	2111.749	1407.794	2182.261	484.835	2245.871	-37.842
3200	901.395	2140.338	1430.241	2272.311	484.370	2302.696	-37.587
3300	903.076	2168.102	1452.182	2362.535	483.639	2359.574	-37.348
3400	904.622	2195.085	1473.637	2452.921	482.617	2416.402	-37.123
3500	906.045	2221.328	1494.627	2543.456	481.308	2473.249	-36.910
3600	907.359	2246.871	1515.169	2634.127	479.732	2530.213	-36.712
3700	908.574	2271.748	1535.282	2724.924	477.862	2587.241	-36.525
3800	909.700	2295.994	1554.984	2815.839	475.673	2644.270	-36.347
3900	910.746	2319.637	1574.288	2906.862	473.203	2701.315	-36.179
4000	911.718	2342.708	1593.211	2997.985	470.437	2758.550	-36.022
4100	912.623	2365.232	1611.768	3089.203	467.344	2815.792	-35.873
4200	913.467	2387.234	1629.970	3180.508	463.947	2873.106	-35.732
4300	914.255	2408.738	1647.832	3271.894	460.236	2930.424	-35.597
4400	914.993	2429.764	1665.365	3363.357	456.218	2987.914	-35.470
4500	915.684	2450.335	1682.581	3454.891	451.905	3045.549	-35.351
4600	916.333	2470.468	1699.491	3546.493	447.252	3103.289	-35.238
4700	916.942	2490.181	1716.105	3638.157	442.272	3161.034	-35.130
4800	917.514	2509.492	1732.434	3729.880	437.006	3218.981	-35.029
4900	918.054	2528.416	1748.486	3821.658	431.389	3276.922	-34.932
5000	918.562	2546.968	1764.270	3913.489	425.503	3335.146	-34.841

3.212. Indeno[7,1-*ab*]naphthacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 16683-71-9
Point Group: C_s

Length: 16.39 Å
Width: 9.128 Å
Breadth: 3.887 Å
L/B Ratio: 1.796

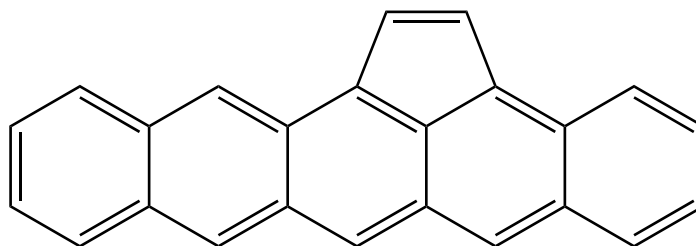
Cartesian coordinates:

C	-3.4095	0.0035	0.0000	C	1.4087	-0.4841	0.0000	H	7.1589	-1.4988	0.0000
C	-3.3018	1.4502	0.0000	C	1.5280	0.9322	0.0000	H	7.3674	0.9668	0.0000
C	-4.6916	1.9386	0.0000	C	0.3493	1.7279	0.0000	H	5.3406	2.4064	0.0000
C	-5.5450	0.8781	0.0000	C	0.1120	-1.0676	0.0000	H	4.9191	-2.5776	0.0000
C	-4.7721	-0.3757	0.0000	C	-1.0176	-0.2872	0.0000	H	2.8933	2.6141	0.0000
C	6.2447	-0.8962	0.0000	C	-0.9013	1.1538	0.0000	H	2.4707	-2.3714	0.0000
C	6.3650	0.5263	0.0000	C	-2.0785	2.0151	0.0000	H	0.4573	2.8202	0.0000
C	5.2583	1.3136	0.0000	C	-2.3479	-0.8803	0.0000	H	0.0180	-2.1629	0.0000
C	5.0215	-1.4865	0.0000	C	-5.0780	-1.7202	0.0000	H	-1.9342	3.1011	0.0000
C	3.8266	-0.6906	0.0000	C	-4.0121	-2.6413	0.0000	H	-6.1141	-2.0711	0.0000
C	3.9467	0.7295	0.0000	C	-2.6814	-2.2490	0.0000	H	-4.2490	-3.7110	0.0000
C	2.8022	1.5209	0.0000	H	-4.9532	2.9948	0.0000	H	-1.8770	-2.9954	0.0000
C	2.5654	-1.2785	0.0000	H	-6.6328	0.9084	0.0000				

Table 3.212: Table of thermodynamic data as a function of temperature for Indeno[7,1-*ab*]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-45.113	477.791	477.791	∞
100	98.533	338.248	727.094	-38.885	500.967	539.936	-282.028
200	194.308	434.205	556.679	-24.495	488.674	583.804	-152.471
250	250.510	483.554	537.093	-13.385	482.909	608.254	-127.085
298.15	305.297	532.375	532.375	0.000	477.791	632.873	-110.874
300	307.374	534.270	532.381	0.567	477.603	633.833	-110.358
350	361.931	585.792	536.325	17.314	472.903	660.255	-98.536
400	412.405	637.468	545.740	36.691	468.833	687.296	-89.750
450	458.044	688.726	558.786	58.473	465.316	714.819	-82.972
500	498.783	739.136	574.309	82.414	462.271	742.726	-77.591
600	567.023	836.355	609.955	135.840	457.323	799.308	-69.585
700	620.962	927.971	648.911	195.342	453.707	856.615	-63.920
800	664.231	1013.816	689.218	259.678	451.268	914.343	-59.699
900	699.509	1094.156	729.797	327.923	449.854	972.309	-56.430
1000	728.670	1169.413	770.036	399.377	449.328	1030.395	-53.821
1100	753.033	1240.039	809.587	473.497	449.520	1088.507	-51.688
1200	773.564	1306.466	848.253	549.856	450.308	1146.557	-49.907
1300	790.989	1369.091	885.932	628.107	451.536	1204.534	-48.398
1400	805.870	1428.269	922.576	707.969	453.090	1262.406	-47.100
1500	818.652	1484.315	958.174	789.211	454.900	1320.159	-45.971
1600	829.688	1537.510	992.734	871.641	456.854	1377.778	-44.979
1700	839.267	1588.104	1026.280	955.100	458.886	1435.251	-44.099
1800	847.619	1636.317	1058.843	1039.454	460.934	1492.660	-43.315
1900	854.936	1682.346	1090.456	1124.590	462.970	1549.909	-42.609
2000	861.374	1726.365	1121.159	1210.412	464.946	1607.076	-41.972
2100	867.063	1768.532	1150.990	1296.839	466.796	1664.133	-41.392
2200	872.110	1808.987	1179.985	1383.803	468.518	1721.108	-40.863
2300	876.604	1847.855	1208.184	1471.243	470.109	1778.007	-40.379
2400	880.621	1885.249	1235.621	1559.108	471.507	1834.798	-39.933
2500	884.224	1921.272	1262.331	1647.353	472.723	1891.635	-39.523
2600	887.465	1956.016	1288.347	1735.941	473.724	1948.324	-39.141
2700	890.392	1989.565	1313.700	1824.836	474.515	2005.042	-38.789
2800	893.041	2021.995	1338.421	1914.010	475.074	2061.754	-38.462
2900	895.447	2053.376	1362.536	2003.436	475.374	2118.404	-38.156
3000	897.637	2083.771	1386.073	2093.092	475.455	2175.070	-37.871
3100	899.636	2113.237	1409.057	2182.957	475.248	2231.671	-37.603
3200	901.465	2141.829	1431.512	2273.013	474.791	2288.347	-37.353
3300	903.142	2169.594	1453.459	2363.245	474.066	2345.076	-37.119
3400	904.684	2196.579	1474.921	2453.637	473.051	2401.755	-36.898
3500	906.105	2222.824	1495.916	2544.178	471.748	2458.452	-36.690
3600	907.416	2248.369	1516.465	2634.855	470.178	2515.267	-36.495
3700	908.628	2273.248	1536.583	2725.658	468.313	2572.145	-36.311
3800	909.752	2297.494	1556.290	2816.577	466.130	2629.024	-36.138
3900	910.795	2321.139	1575.599	2907.605	463.665	2685.919	-35.973
4000	911.764	2344.211	1594.527	2998.734	460.903	2743.004	-35.819
4100	912.667	2366.736	1613.088	3089.956	457.814	2800.095	-35.673
4200	913.510	2388.739	1631.295	3181.265	454.423	2857.258	-35.534
4300	914.296	2410.244	1649.161	3272.656	450.715	2914.427	-35.403
4400	915.032	2431.272	1666.698	3364.123	446.701	2971.766	-35.279
4500	915.722	2451.843	1683.918	3455.661	442.392	3029.250	-35.162
4600	916.369	2471.977	1700.832	3547.266	437.743	3086.839	-35.051
4700	916.976	2491.691	1717.450	3638.933	432.767	3144.433	-34.946
4800	917.548	2511.002	1733.781	3730.660	427.504	3202.229	-34.847
4900	918.086	2529.927	1749.837	3822.442	421.890	3260.019	-34.752
5000	918.593	2548.480	1765.625	3914.276	416.007	3318.092	-34.663

3.213. Cyclopenta[fg]pentacene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 908069-55-6
Point Group: C_s

Length: 16.53 Å
Width: 8.587 Å
Breadth: 3.883 Å
L/B Ratio: 1.925

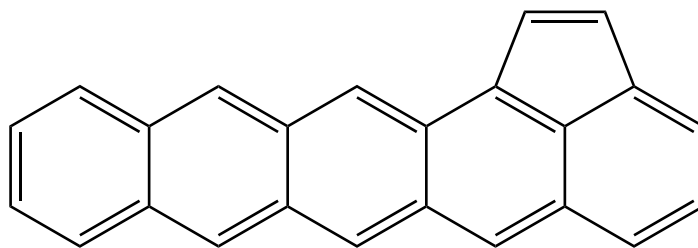
Cartesian coordinates:

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C	-3.5388	1.0046	0.0000	C	3.7656	0.8382	0.0000	H	5.0901	2.5740	0.0000
C	-4.8215	1.6651	0.0000	C	3.7103	-0.5953	0.0000	H	4.8946	-2.4288	0.0000
C	-5.9755	0.9557	0.0000	C	2.4895	-1.2366	0.0000	H	2.6455	2.6710	0.0000
C	-5.9548	-0.4761	0.0000	C	5.0574	1.4786	0.0000	H	2.4351	-2.3325	0.0000
C	-2.3743	1.7572	0.0000	C	6.1945	0.7431	0.0000	H	0.2405	2.8202	0.0000
C	-1.1030	1.1218	0.0000	C	6.1387	-0.6889	0.0000	H	-2.4222	2.8528	0.0000
C	-1.1205	-0.2812	0.0000	C	4.9479	-1.3341	0.0000	H	-4.8359	2.7613	0.0000
C	-2.3046	-1.0788	0.0000	C	-0.4732	-2.4858	0.0000	H	-6.9465	1.4616	0.0000
C	0.1599	1.7264	0.0000	C	-1.8396	-2.4715	0.0000	H	-6.9102	-1.0111	0.0000
C	1.3283	0.9411	0.0000	H	0.1756	-3.3594	0.0000	H	-4.7461	-2.2448	0.0000
C	1.2821	-0.4975	0.0000	H	-2.5074	-3.3306	0.0000				

Table 3.213: Table of thermodynamic data as a function of temperature for Cyclopenta[fg]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-45.220	522.450	522.450	∞
100	99.025	335.285	725.802	-39.052	545.458	584.723	-305.422
200	195.247	431.796	554.693	-24.579	533.248	628.859	-164.238
250	251.378	481.349	535.045	-13.424	527.528	653.424	-136.523
298.15	306.052	530.313	530.313	0.000	522.450	678.146	-118.806
300	308.125	532.213	530.319	0.568	522.263	679.110	-118.241
350	362.568	583.842	534.272	17.350	517.597	705.631	-105.308
400	412.950	635.597	543.705	36.757	513.557	732.768	-95.688
450	458.518	686.914	556.772	58.564	510.066	760.383	-88.261
500	499.203	737.372	572.318	82.527	507.042	788.380	-82.360
600	567.360	834.660	608.008	135.991	502.132	845.134	-73.574
700	621.234	926.322	647.003	195.523	498.546	902.608	-67.352
800	664.450	1012.199	687.345	259.884	496.131	960.500	-62.713
900	699.684	1092.563	727.954	328.148	494.738	1018.626	-59.118
1000	728.809	1167.836	768.219	399.617	494.227	1076.871	-56.249
1100	753.144	1238.474	807.792	473.751	494.431	1135.139	-53.902
1200	773.652	1304.911	846.478	550.119	495.230	1193.346	-51.944
1300	791.059	1367.542	884.174	628.378	496.466	1251.477	-50.284
1400	805.927	1426.724	920.834	708.246	498.026	1309.504	-48.857
1500	818.697	1482.773	956.445	789.493	499.841	1367.412	-47.617
1600	829.725	1535.972	991.017	871.928	501.798	1425.185	-46.527
1700	839.296	1586.567	1024.573	955.390	503.835	1482.811	-45.560
1800	847.643	1634.782	1057.145	1039.746	505.885	1540.374	-44.700
1900	854.956	1680.812	1088.767	1124.884	507.923	1597.777	-43.925
2000	861.391	1724.832	1119.478	1210.708	509.901	1655.096	-43.226
2100	867.077	1767.000	1149.316	1297.137	511.752	1712.307	-42.590
2200	872.121	1807.455	1178.318	1384.102	513.476	1769.436	-42.011
2300	876.613	1846.324	1206.522	1471.543	515.068	1826.488	-41.480
2400	880.629	1883.718	1233.964	1559.409	516.467	1883.432	-40.991
2500	884.230	1919.742	1260.680	1647.655	517.683	1940.421	-40.542
2600	887.471	1954.486	1286.700	1736.243	518.685	1997.263	-40.125
2700	890.396	1988.035	1312.058	1825.139	519.477	2054.134	-39.739
2800	893.045	2020.465	1336.782	1914.313	520.036	2111.000	-39.380
2900	895.450	2051.846	1360.901	2003.740	520.336	2167.803	-39.046
3000	897.640	2082.241	1384.442	2093.396	520.418	2224.622	-38.733
3100	899.638	2111.707	1407.430	2183.261	520.211	2281.376	-38.440
3200	901.467	2140.299	1429.887	2273.318	519.754	2338.205	-38.166
3300	903.144	2168.065	1451.838	2363.550	519.029	2395.087	-37.910
3400	904.686	2195.049	1473.302	2453.942	518.014	2451.919	-37.668
3500	906.106	2221.295	1494.300	2544.483	516.711	2508.769	-37.441
3600	907.417	2246.839	1514.850	2635.160	515.141	2565.737	-37.227
3700	908.629	2271.718	1534.972	2725.963	513.276	2622.768	-37.026
3800	909.753	2295.965	1554.680	2816.883	511.093	2679.799	-36.836
3900	910.795	2319.610	1573.992	2907.911	508.628	2736.847	-36.655
4000	911.765	2342.682	1592.922	2999.039	505.867	2794.085	-36.486
4100	912.668	2365.207	1611.484	3090.261	502.778	2851.329	-36.326
4200	913.510	2387.210	1629.693	3181.571	499.386	2908.645	-36.174
4300	914.297	2408.715	1647.561	3272.962	495.679	2965.967	-36.029
4400	915.033	2429.742	1665.100	3364.428	491.665	3023.459	-35.892
4500	915.722	2450.314	1682.321	3455.966	487.356	3081.095	-35.764
4600	916.369	2470.447	1699.236	3547.571	482.707	3138.838	-35.642
4700	916.976	2490.161	1715.855	3639.239	477.731	3196.584	-35.525
4800	917.548	2509.473	1732.188	3730.965	472.468	3254.534	-35.416
4900	918.086	2528.398	1748.245	3822.747	466.854	3312.476	-35.311
5000	918.593	2546.951	1764.034	3914.582	460.971	3370.703	-35.213

3.214. Cyclopenta[de]pentacene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 16683-65-1
Point Group: C_s

Length: 16.53 Å
Width: 8.585 Å
Breadth: 3.884 Å
L/B Ratio: 1.925

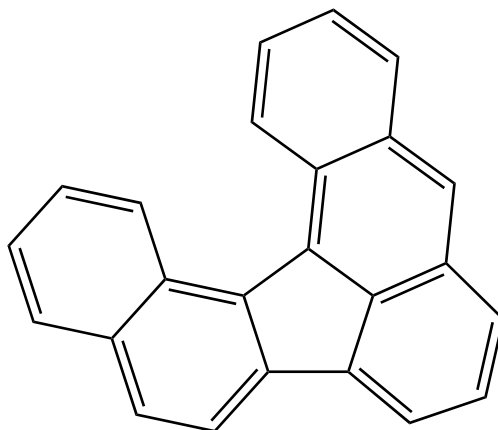
Cartesian coordinates:

C	-5.7645	-0.2613	0.0000	C	0.2062	-1.1909	0.0000	H	7.2481	-1.4578	0.0000
C	-4.5830	-0.9249	0.0000	C	2.8318	1.4626	0.0000	H	7.4004	1.0100	0.0000
C	-3.3573	-0.1554	0.0000	C	3.9805	0.7015	0.0000	H	5.3441	2.4065	0.0000
C	-3.3086	1.2536	0.0000	C	3.8920	-0.7313	0.0000	H	5.0356	-2.5909	0.0000
C	-4.5933	1.9102	0.0000	C	2.6584	-1.3455	0.0000	H	2.8938	2.5579	0.0000
C	-5.7425	1.1806	0.0000	C	5.2869	1.3120	0.0000	H	2.5843	-2.4401	0.0000
C	-2.0547	1.8289	0.0000	C	6.4065	0.5508	0.0000	H	0.4579	2.7086	0.0000
C	-0.8814	1.0109	0.0000	C	6.3182	-0.8799	0.0000	H	0.1327	-2.2856	0.0000
C	-0.9607	-0.4274	0.0000	C	5.1135	-1.4978	0.0000	H	-1.9419	2.9196	0.0000
C	-2.2568	-1.0020	0.0000	C	-2.7845	-2.3737	0.0000	H	-4.6170	3.0053	0.0000
C	0.3808	1.6137	0.0000	C	-4.1487	-2.3308	0.0000	H	-6.7109	1.6934	0.0000
C	1.5520	0.8472	0.0000	H	-2.1536	-3.2605	0.0000	H	-6.7280	-0.7801	0.0000
C	1.4644	-0.5774	0.0000	H	-4.8361	-3.1737	0.0000				

Table 3.214: Table of thermodynamic data as a function of temperature for Cyclopenta[de]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-45.241	525.615	525.615	∞
100	98.625	337.316	727.662	-39.035	548.640	587.702	-306.978
200	195.128	433.554	556.554	-24.600	536.393	631.652	-164.967
250	251.608	483.119	536.885	-13.441	530.675	656.130	-137.088
298.15	306.535	532.147	532.147	0.000	525.615	680.764	-119.265
300	308.616	534.049	532.152	0.569	525.429	681.726	-118.697
350	363.219	585.768	536.112	17.379	520.792	708.153	-105.684
400	413.682	637.615	545.562	36.821	516.787	735.191	-96.004
450	459.276	689.021	558.652	58.666	513.333	762.703	-88.530
500	499.954	739.558	574.224	82.667	510.348	790.592	-82.591
600	568.053	836.978	609.972	136.203	505.509	847.121	-73.747
700	621.854	928.742	649.026	195.801	501.989	904.358	-67.483
800	665.000	1014.698	689.422	260.220	499.633	962.003	-62.811
900	700.173	1095.122	730.081	328.537	498.291	1019.877	-59.191
1000	729.246	1170.444	770.392	400.052	497.827	1077.863	-56.301
1100	753.535	1241.122	810.007	474.227	498.073	1135.868	-53.937
1200	774.004	1307.590	848.730	550.632	498.908	1193.809	-51.964
1300	791.377	1370.248	886.460	628.924	500.177	1251.671	-50.292
1400	806.215	1429.453	923.151	708.823	501.768	1309.426	-48.854
1500	818.959	1485.521	958.790	790.098	503.611	1367.060	-47.604
1600	829.964	1538.736	993.387	872.557	505.593	1424.557	-46.506
1700	839.515	1589.345	1026.968	956.042	507.652	1481.906	-45.532
1800	847.844	1637.572	1059.561	1040.419	509.723	1539.191	-44.665
1900	855.140	1683.612	1091.203	1125.576	511.780	1596.314	-43.885
2000	861.560	1727.642	1121.932	1211.418	513.776	1653.353	-43.180
2100	867.233	1769.817	1151.787	1297.864	515.644	1710.282	-42.540
2200	872.266	1810.280	1180.805	1384.844	517.382	1767.129	-41.956
2300	876.748	1849.154	1209.024	1472.299	518.988	1823.898	-41.421
2400	880.754	1886.554	1236.480	1560.177	520.400	1880.559	-40.928
2500	884.347	1922.583	1263.208	1648.436	521.629	1937.264	-40.476
2600	887.580	1957.331	1289.241	1737.035	522.642	1993.822	-40.056
2700	890.499	1990.885	1314.610	1825.941	523.444	2050.408	-39.667
2800	893.141	2023.319	1339.345	1915.125	524.013	2106.989	-39.306
2900	895.540	2054.703	1363.475	2004.561	524.323	2163.506	-38.968
3000	897.724	2085.100	1387.025	2094.226	524.413	2220.040	-38.654
3100	899.718	2114.569	1410.021	2184.100	524.215	2276.507	-38.358
3200	901.542	2143.163	1432.487	2274.164	523.765	2333.050	-38.082
3300	903.215	2170.931	1454.446	2364.403	523.048	2389.646	-37.824
3400	904.753	2197.918	1475.917	2454.803	522.040	2446.191	-37.580
3500	906.170	2224.166	1496.923	2545.350	520.744	2502.754	-37.351
3600	907.478	2249.712	1517.480	2636.033	519.180	2559.434	-37.136
3700	908.687	2274.592	1537.608	2726.842	517.321	2616.178	-36.933
3800	909.807	2298.841	1557.323	2817.768	515.144	2672.922	-36.741
3900	910.848	2322.487	1576.640	2908.801	512.684	2729.683	-36.559
4000	911.815	2345.560	1595.576	2999.935	509.928	2786.632	-36.389
4100	912.715	2368.086	1614.144	3091.162	506.844	2843.589	-36.227
4200	913.555	2390.091	1632.358	3182.476	503.457	2900.617	-36.074
4300	914.340	2411.596	1650.231	3273.871	499.754	2957.650	-35.928
4400	915.074	2432.625	1667.774	3365.342	495.744	3014.854	-35.790
4500	915.762	2453.197	1685.001	3456.884	491.439	3072.202	-35.660
4600	916.407	2473.332	1701.920	3548.493	486.794	3129.657	-35.538
4700	917.013	2493.047	1718.544	3640.164	481.821	3187.115	-35.420
4800	917.583	2512.359	1734.881	3731.894	476.562	3244.775	-35.310
4900	918.120	2531.284	1750.942	3823.680	470.952	3302.429	-35.204
5000	918.625	2549.838	1766.735	3915.517	465.072	3360.367	-35.105

3.215. Naphth[1,2-*a*]aceanthrylene



Other names: Dibenzo[*a,l*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 908069-62-5

Point Group: C₁

Length: 13.33 Å

Width: 11.88 Å

Breadth: 4.739 Å

L/B Ratio: 1.122

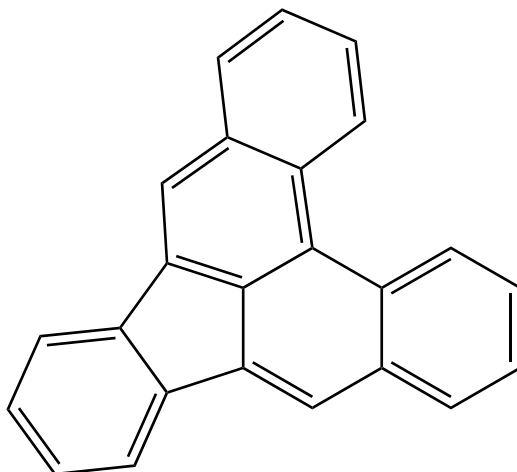
Cartesian coordinates:

C	1.3026	-3.7233	0.4667	C	0.5621	2.2683	0.0484	H	4.4279	-2.5612	-0.2546
C	2.6987	-3.7344	0.1921	C	-0.8569	0.3986	0.0420	H	-0.4743	-2.5604	0.6560
C	3.3481	-2.5691	-0.0643	C	-0.8213	1.8059	0.1570	H	4.4756	-0.1833	-0.3720
C	0.5978	-2.5615	0.4174	C	-1.9725	2.5839	0.3363	H	4.4438	2.4513	-0.3436
C	1.2217	-1.3154	0.0921	C	-3.1905	1.9535	0.3685	H	3.0776	4.5081	-0.1549
C	2.6470	-1.3164	-0.0811	C	-2.1236	-0.2307	-0.0778	H	0.6102	4.4163	0.1215
C	3.3884	-0.1379	-0.2373	C	-3.2850	0.5575	0.1368	H	-1.8822	3.6688	0.4537
C	2.7409	1.0993	-0.1882	C	-4.5706	-0.0523	0.0782	H	-4.1085	2.5260	0.5444
C	3.3557	2.3930	-0.2315	C	-4.7032	-1.3715	-0.2509	H	-5.4536	0.5613	0.2916
C	2.5964	3.5243	-0.1265	C	-3.5554	-2.1382	-0.5577	H	-5.6903	-1.8423	-0.2962
C	1.1748	3.4833	0.0262	C	-2.3088	-1.5837	-0.4744	H	-3.6791	-3.1802	-0.8706
C	0.5432	-0.0912	-0.0004	H	0.8088	-4.6657	0.7259	H	-1.4276	-2.1809	-0.7433
C	1.3478	1.0714	-0.0687	H	3.2346	-4.6889	0.2054				

Table 3.215: Table of thermodynamic data as a function of temperature for Naphth[1,2-*a*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.829	470.272	470.272	∞
100	98.344	332.914	720.045	-38.713	493.619	533.121	-278.468
200	193.489	428.668	550.449	-24.356	481.294	577.531	-150.832
250	249.052	477.764	530.978	-13.304	475.470	602.264	-125.833
298.15	303.423	526.288	526.288	0.000	470.272	627.168	-109.875
300	305.490	528.172	526.294	0.563	470.080	628.140	-109.367
350	359.856	579.387	530.215	17.210	465.280	654.874	-97.733
400	410.310	630.782	539.575	36.483	461.106	682.243	-89.090
450	456.026	681.797	552.549	58.162	457.486	710.106	-82.425
500	496.890	732.001	567.992	82.005	454.343	738.365	-77.135
600	565.411	828.900	603.474	135.256	449.219	795.677	-69.268
700	619.602	920.287	642.273	194.610	445.455	853.742	-63.706
800	663.074	1005.964	682.438	258.820	442.890	912.247	-59.562
900	698.513	1086.177	722.891	326.958	441.370	971.005	-56.355
1000	727.802	1161.336	763.018	398.318	440.750	1029.894	-53.795
1100	752.270	1231.885	802.468	472.358	440.861	1088.817	-51.703
1200	772.888	1298.250	841.046	548.644	441.577	1147.687	-49.956
1300	790.385	1360.823	878.645	626.831	442.741	1206.487	-48.476
1400	805.328	1419.958	915.218	706.636	444.238	1265.188	-47.204
1500	818.162	1475.969	950.751	787.827	445.997	1323.775	-46.097
1600	829.245	1529.134	985.253	870.210	447.903	1382.230	-45.124
1700	838.863	1579.702	1018.745	953.627	449.894	1440.542	-44.262
1800	847.250	1627.893	1051.259	1037.942	451.903	1498.792	-43.493
1900	854.598	1673.903	1082.828	1123.042	453.903	1556.885	-42.801
2000	861.064	1717.906	1113.490	1208.832	455.847	1614.896	-42.176
2100	866.777	1760.058	1143.282	1295.230	457.667	1672.800	-41.608
2200	871.845	1800.500	1172.243	1382.166	459.362	1730.624	-41.089
2300	876.359	1839.356	1200.408	1469.581	460.928	1788.372	-40.614
2400	880.393	1876.741	1227.815	1557.422	462.302	1846.013	-40.177
2500	884.011	1912.755	1254.497	1645.645	463.495	1903.701	-39.775
2600	887.267	1947.491	1280.486	1734.212	464.476	1961.242	-39.401
2700	890.207	1981.033	1305.815	1823.088	465.248	2018.813	-39.055
2800	892.868	2013.456	1330.512	1912.244	465.789	2076.379	-38.735
2900	895.284	2044.831	1354.606	2001.654	466.073	2133.883	-38.435
3000	897.484	2075.220	1378.122	2091.294	466.138	2191.404	-38.155
3100	899.492	2104.682	1401.087	2181.144	465.916	2248.860	-37.892
3200	901.329	2133.269	1423.523	2271.186	465.444	2306.392	-37.647
3300	903.014	2161.031	1445.453	2361.405	464.707	2363.977	-37.418
3400	904.563	2188.011	1466.898	2451.785	463.679	2421.513	-37.201
3500	905.989	2214.253	1487.878	2542.313	462.364	2479.066	-36.997
3600	907.306	2239.795	1508.412	2632.979	460.783	2536.739	-36.806
3700	908.524	2264.671	1528.516	2723.771	458.907	2594.474	-36.627
3800	909.653	2288.915	1548.209	2814.681	456.714	2652.211	-36.456
3900	910.701	2312.557	1567.506	2905.699	454.239	2709.964	-36.295
4000	911.675	2335.626	1586.422	2996.819	451.468	2767.907	-36.144
4100	912.582	2358.149	1604.971	3088.032	448.371	2825.857	-36.001
4200	913.428	2380.151	1623.167	3179.333	444.971	2883.879	-35.866
4300	914.218	2401.653	1641.022	3270.716	441.256	2941.906	-35.736
4400	914.958	2422.679	1658.549	3362.175	437.234	3000.105	-35.615
4500	915.650	2443.249	1675.759	3453.705	432.917	3058.448	-35.501
4600	916.300	2463.381	1692.663	3545.303	428.261	3116.897	-35.393
4700	916.910	2483.094	1709.272	3636.964	423.278	3175.350	-35.289
4800	917.484	2502.404	1725.595	3728.684	418.009	3234.006	-35.192
4900	918.025	2521.327	1741.642	3820.460	412.389	3292.656	-35.099
5000	918.534	2539.879	1757.422	3912.288	406.500	3351.589	-35.013

3.216. Dibenz[*a,e*]acephenanthrylene



Other names: Dibenzo[*b,e*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 2997-45-7

Point Group: C₂

Length: 13.72 Å

Width: 12.06 Å

Breadth: 4.393 Å

L/B Ratio: 1.137

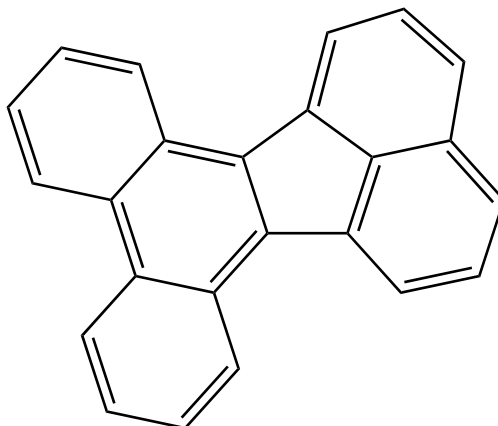
Cartesian coordinates:

C	-5.0129	-0.6915	-0.0599	C	2.9675	1.5184	-0.2983	H	-3.8180	2.5023	0.2151
C	-5.0130	0.6912	0.0599	C	-1.2351	-1.1746	-0.0901	H	-3.8179	-2.5025	-0.2151
C	-3.8142	1.4118	0.1214	C	-0.4057	-0.0000	0.0000	H	-1.2421	3.3119	0.2957
C	-3.8141	-1.4120	-0.1214	C	0.9744	0.0000	0.0000	H	0.7360	4.6309	0.2733
C	-2.6264	-0.7110	-0.0603	C	-0.6537	-2.3940	-0.1859	H	3.1844	4.9003	-0.0435
C	-2.6265	0.7108	0.0603	C	0.7801	-2.4688	-0.1025	H	4.5950	2.9027	-0.4923
C	-1.2352	1.1745	0.0901	C	1.5915	-1.3137	0.0460	H	3.6134	0.6609	-0.5271
C	-0.6539	2.3940	0.1859	C	2.9677	-1.5183	0.2984	H	-1.2418	-3.3120	-0.2957
C	1.5914	1.3138	-0.0460	C	3.5247	-2.7752	0.2997	H	3.6138	-0.6610	0.5273
C	0.7799	2.4688	0.1025	C	2.7271	-3.9059	0.0625	H	4.5952	-2.9026	0.4924
C	1.3746	3.7527	0.1204	C	1.3749	-3.7527	-0.1205	H	3.1847	-4.9001	0.0433
C	2.7268	3.9060	-0.0626	H	-5.9644	-1.2316	-0.1070	H	0.7364	-4.6308	-0.2735
C	3.5245	2.7753	-0.2997	H	-5.9644	1.2313	0.1069				

Table 3.216: Table of thermodynamic data as a function of temperature for Dibenz[*a,e*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.791	427.065	427.065	∞
100	99.269	327.696	714.128	-38.643	450.482	490.506	-256.209
200	192.987	423.683	544.989	-24.261	438.181	535.415	-139.833
250	248.037	472.605	525.597	-13.248	432.319	560.401	-117.087
298.15	302.162	520.927	520.927	0.000	427.065	585.559	-102.585
300	304.222	522.803	520.933	0.561	426.871	586.541	-102.124
350	358.503	573.815	524.838	17.142	422.005	613.549	-91.565
400	408.960	625.029	534.162	36.347	417.763	641.201	-83.730
450	454.724	675.888	547.089	57.959	414.076	669.356	-77.695
500	495.656	725.958	562.481	81.738	410.869	697.914	-72.909
600	564.329	822.645	597.855	134.874	405.630	755.841	-65.800
700	618.663	913.876	636.552	194.127	401.765	814.539	-60.780
800	662.259	999.435	676.623	258.250	399.113	873.692	-57.045
900	697.804	1079.559	716.991	326.311	397.516	933.108	-54.155
1000	727.181	1154.648	757.042	397.606	396.830	992.662	-51.850
1100	751.723	1225.141	796.426	471.587	396.882	1052.257	-49.966
1200	772.402	1291.461	834.943	547.822	397.547	1111.803	-48.395
1300	789.953	1353.998	872.488	625.963	398.666	1171.284	-47.062
1400	804.941	1413.103	909.012	705.727	400.122	1230.669	-45.916
1500	817.814	1469.088	944.501	786.881	401.843	1289.943	-44.919
1600	828.931	1522.232	978.962	869.231	403.717	1349.087	-44.042
1700	838.578	1572.782	1012.418	952.618	405.678	1408.090	-43.264
1800	846.991	1620.957	1044.898	1036.906	407.660	1467.033	-42.571
1900	854.361	1666.953	1076.437	1121.981	409.635	1525.820	-41.947
2000	860.847	1710.945	1107.070	1207.749	411.556	1584.527	-41.383
2100	866.577	1753.087	1136.837	1294.126	413.355	1643.128	-40.870
2200	871.661	1793.520	1165.773	1381.042	415.031	1701.649	-40.401
2300	876.188	1832.369	1193.917	1468.439	416.579	1760.095	-39.972
2400	880.235	1869.746	1221.302	1556.264	417.937	1818.436	-39.576
2500	883.865	1905.754	1247.965	1644.472	419.115	1876.823	-39.213
2600	887.131	1940.484	1273.936	1733.025	420.082	1935.065	-38.875
2700	890.079	1974.021	1299.248	1821.888	420.841	1993.337	-38.563
2800	892.748	2006.440	1323.929	1911.031	421.369	2051.604	-38.272
2900	895.172	2037.811	1348.008	2000.429	421.641	2109.810	-38.001
3000	897.378	2068.196	1371.510	2090.059	421.695	2168.033	-37.748
3100	899.392	2097.655	1394.461	2179.899	421.463	2226.192	-37.510
3200	901.235	2126.239	1416.885	2269.931	420.982	2284.427	-37.289
3300	902.926	2153.997	1438.803	2360.141	420.235	2342.715	-37.081
3400	904.479	2180.976	1460.237	2450.512	419.199	2400.954	-36.885
3500	905.911	2207.215	1481.206	2541.032	417.876	2459.212	-36.701
3600	907.232	2232.754	1501.729	2631.690	416.287	2517.588	-36.528
3700	908.453	2257.628	1521.824	2722.475	414.404	2576.028	-36.366
3800	909.586	2281.871	1541.508	2813.378	412.204	2634.468	-36.213
3900	910.636	2305.511	1560.796	2904.390	409.723	2692.926	-36.067
4000	911.613	2328.579	1579.703	2995.503	406.946	2751.574	-35.931
4100	912.523	2351.100	1598.244	3086.710	403.842	2810.229	-35.802
4200	913.372	2373.100	1616.432	3178.006	400.436	2868.956	-35.680
4300	914.165	2394.602	1634.280	3269.383	396.716	2927.688	-35.564
4400	914.907	2415.627	1651.800	3360.837	392.689	2986.591	-35.455
4500	915.601	2436.195	1669.003	3452.363	388.367	3045.640	-35.352
4600	916.253	2456.326	1685.901	3543.956	383.706	3104.794	-35.255
4700	916.866	2476.038	1702.503	3635.612	378.719	3163.953	-35.163
4800	917.441	2495.347	1718.821	3727.328	373.445	3223.315	-35.076
4900	917.983	2514.270	1734.862	3819.099	367.821	3282.670	-34.993
5000	918.494	2532.821	1750.636	3910.923	361.928	3342.309	-34.916

3.217. Dibenzo[*j,l*]fluoranthene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 203-18-9
Point Group: C_{2v}

Length: 13.01 Å
Width: 11.49 Å
Breadth: 3.886 Å
L/B Ratio: 1.133

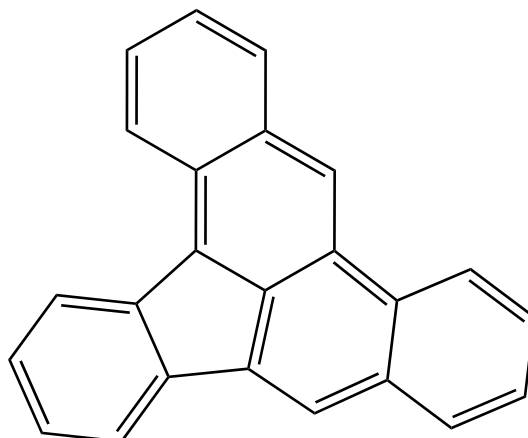
Cartesian coordinates:

C	4.2046	1.4936	0.0000	C	-2.3355	-0.8433	0.0000	H	1.3437	3.4037	0.0000
C	3.3802	2.5936	0.0000	C	-3.5098	-1.6301	0.0000	H	1.6821	-3.2503	0.0000
C	1.9614	2.4947	0.0000	C	-3.4418	-3.0031	0.0000	H	4.1664	-3.1906	0.0000
C	3.6449	0.1852	0.0000	C	-2.1933	-3.6482	0.0000	H	5.4295	-1.0622	0.0000
C	2.2041	-2.2831	0.0000	C	-1.0353	-2.9078	0.0000	H	-4.4846	-1.1188	0.0000
C	3.6256	-2.2377	0.0000	C	-2.4089	0.6023	0.0000	H	-4.3584	-3.6020	0.0000
C	4.3344	-1.0598	0.0000	C	-1.2304	1.3783	0.0000	H	-2.1514	-4.7422	0.0000
C	2.2585	0.1147	0.0000	C	-1.3249	2.7881	0.0000	H	-0.0536	-3.4050	0.0000
C	1.3913	1.2504	0.0000	C	-2.5522	3.4071	0.0000	H	-0.3992	3.3831	0.0000
C	1.5108	-1.1031	0.0000	C	-3.7288	2.6387	0.0000	H	-2.6215	4.4997	0.0000
C	0.0962	-0.6931	0.0000	C	-3.6570	1.2658	0.0000	H	-4.7014	3.1414	0.0000
C	0.0254	0.6994	0.0000	H	5.2939	1.6070	0.0000	H	-4.5749	0.6582	0.0000
C	-1.0844	-1.4957	0.0000	H	3.8216	3.5964	0.0000				

Table 3.217: Table of thermodynamic data as a function of temperature for Dibenzo[*j,l*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-45.441	441.158	441.158	∞
100	101.144	341.574	730.467	-38.889	464.328	502.965	-262.716
200	194.212	438.567	560.395	-24.366	452.170	546.427	-142.709
250	249.100	487.747	540.926	-13.295	446.365	570.662	-119.231
298.15	303.038	536.240	536.240	0.000	441.158	595.086	-104.255
300	305.091	538.121	536.246	0.563	440.965	596.040	-103.778
350	359.192	589.253	540.161	17.182	436.138	622.279	-92.868
400	409.505	640.550	549.505	36.418	431.927	649.156	-84.769
450	455.156	691.465	562.455	58.055	428.264	676.534	-78.528
500	495.998	741.576	577.870	81.853	425.077	704.312	-73.577
600	564.531	838.313	613.287	135.016	419.864	760.675	-66.221
700	618.751	929.566	652.019	194.283	416.013	817.805	-61.024
800	662.254	1015.131	692.119	258.410	413.365	875.388	-57.156
900	697.724	1095.250	732.509	326.467	411.764	933.234	-54.162
1000	727.046	1170.327	772.577	397.750	411.068	991.221	-51.775
1100	751.550	1240.805	811.973	471.716	411.104	1049.248	-49.824
1200	772.205	1307.109	850.499	547.932	411.751	1107.228	-48.195
1300	789.740	1369.630	888.051	626.053	412.849	1165.146	-46.815
1400	804.722	1428.719	924.579	705.795	414.283	1222.968	-45.629
1500	817.594	1484.689	960.071	786.927	415.983	1280.681	-44.596
1600	828.713	1537.819	994.534	869.256	417.834	1338.266	-43.689
1700	838.366	1588.355	1027.990	952.621	419.774	1395.711	-42.884
1800	846.786	1636.519	1060.470	1036.888	421.735	1453.097	-42.167
1900	854.164	1682.504	1092.008	1121.943	423.690	1510.328	-41.521
2000	860.658	1726.486	1122.640	1207.691	425.592	1567.481	-40.938
2100	866.397	1768.619	1152.405	1294.050	427.373	1624.528	-40.407
2200	871.490	1809.044	1181.339	1380.949	429.031	1681.496	-39.923
2300	876.026	1847.885	1209.481	1468.329	430.562	1738.391	-39.479
2400	880.081	1885.255	1236.864	1556.138	431.904	1795.180	-39.070
2500	883.718	1921.257	1263.525	1644.331	433.067	1852.017	-38.695
2600	886.991	1955.982	1289.494	1732.870	434.019	1908.708	-38.346
2700	889.947	1989.514	1314.803	1821.719	434.765	1965.431	-38.023
2800	892.623	2021.928	1339.482	1910.850	435.281	2022.149	-37.723
2900	895.053	2053.295	1363.558	2000.235	435.540	2078.806	-37.443
3000	897.265	2083.676	1387.058	2089.853	435.583	2135.481	-37.181
3100	899.285	2113.131	1410.007	2179.682	435.340	2192.092	-36.936
3200	901.133	2141.711	1432.429	2269.704	434.848	2248.779	-36.707
3300	902.828	2169.467	1454.345	2359.904	434.091	2305.521	-36.493
3400	904.386	2196.443	1475.776	2450.265	433.045	2362.213	-36.290
3500	905.822	2222.680	1496.743	2540.777	431.713	2418.924	-36.100
3600	907.147	2248.216	1517.265	2631.426	430.116	2475.754	-35.922
3700	908.373	2273.088	1537.358	2722.203	428.225	2532.648	-35.754
3800	909.508	2297.328	1557.039	2813.098	426.016	2589.543	-35.595
3900	910.562	2320.967	1576.325	2904.102	423.527	2646.454	-35.445
4000	911.542	2344.033	1595.231	2995.208	420.743	2703.557	-35.304
4100	912.455	2366.552	1613.770	3086.408	417.633	2760.666	-35.171
4200	913.307	2388.551	1631.956	3177.697	414.220	2817.848	-35.044
4300	914.102	2410.051	1649.802	3269.067	410.493	2875.035	-34.924
4400	914.847	2431.074	1667.321	3360.515	406.460	2932.394	-34.811
4500	915.544	2451.641	1684.522	3452.035	402.133	2989.898	-34.705
4600	916.198	2471.771	1701.418	3543.623	397.466	3047.508	-34.605
4700	916.812	2491.482	1718.019	3635.273	392.473	3105.122	-34.509
4800	917.390	2510.790	1734.335	3726.984	387.195	3162.940	-34.419
4900	917.934	2529.711	1750.375	3818.750	381.565	3220.751	-34.333
5000	918.447	2548.261	1766.147	3910.570	375.667	3278.846	-34.253

3.218. Dibenz[*a,e*]aceanthrylene



Other names: Dibenzo[*a,e*]fluoranthene
2,3,5,6-Dibenzofluoranthene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 5385-75-1
Point Group: C_s

Length: 13.85 Å
Width: 12.08 Å
Breadth: 3.895 Å
L/B Ratio: 1.147

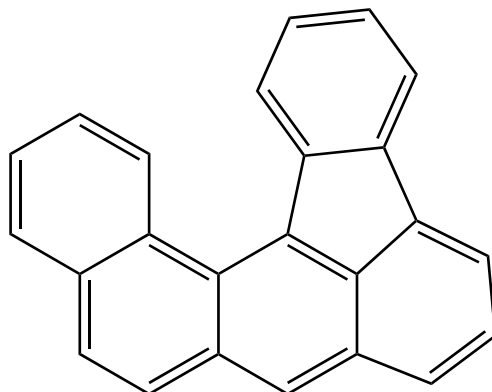
Cartesian coordinates:

C	4.9465	-0.1620	0.0000	C	-1.8742	-4.4053	0.0000	H	3.9486	3.0950	0.0000
C	5.0288	1.2352	0.0000	C	-0.5996	-3.9216	0.0000	H	3.6273	-1.8780	0.0000
C	3.8795	2.0009	0.0000	C	0.1218	0.1839	0.0000	H	1.5391	3.3151	0.0000
C	3.7128	-0.7820	0.0000	C	0.2101	1.6324	0.0000	H	1.8223	-2.7379	0.0000
C	2.5328	-0.0203	0.0000	C	-1.2091	-0.2500	0.0000	H	-3.6359	-1.4656	0.0000
C	2.6111	1.3910	0.0000	C	-2.0425	0.9599	0.0000	H	-3.9955	-3.9373	0.0000
C	1.4230	2.2256	0.0000	C	-1.1808	2.1025	0.0000	H	-2.0614	-5.4841	0.0000
C	1.2326	-0.6675	0.0000	C	-1.7057	3.3787	0.0000	H	0.2579	-4.6044	0.0000
C	0.9776	-2.0338	0.0000	C	-3.0983	3.5245	0.0000	H	-1.0499	4.2550	0.0000
C	-0.3501	-2.5139	0.0000	C	-3.9353	2.4173	0.0000	H	-3.5304	4.5307	0.0000
C	-1.4689	-1.6293	0.0000	C	-3.4144	1.1187	0.0000	H	-5.0212	2.5580	0.0000
C	-2.7888	-2.1695	0.0000	H	5.8635	-0.7602	0.0000	H	-4.0712	0.2369	0.0000
C	-2.9839	-3.5185	0.0000	H	6.0110	1.7193	0.0000				

Table 3.218: Table of thermodynamic data as a function of temperature for Dibenz[*a,e*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.297	423.533	423.533	∞
100	101.171	338.229	727.743	-38.951	446.642	485.613	-253.653
200	194.517	435.380	557.398	-24.403	434.508	529.402	-138.263
250	249.487	484.636	537.899	-13.316	428.720	553.795	-115.707
298.15	303.517	533.206	533.206	0.000	423.533	578.367	-101.325
300	305.573	535.090	533.212	0.563	423.342	579.326	-100.868
350	359.742	586.301	537.132	17.209	418.540	605.714	-90.396
400	410.086	637.674	546.491	36.473	414.357	632.738	-82.625
450	455.742	688.659	559.460	58.139	410.724	660.257	-76.639
500	496.578	738.831	574.897	81.967	407.566	688.174	-71.892
600	565.091	835.671	610.361	135.186	402.410	744.806	-64.840
700	619.305	927.010	649.140	194.509	398.615	802.196	-59.859
800	662.809	1012.649	689.285	258.691	396.023	860.031	-56.153
900	698.282	1092.834	729.718	326.804	394.477	918.122	-53.285
1000	727.602	1167.970	769.827	398.143	393.836	976.347	-50.998
1100	752.098	1238.501	809.261	472.164	393.928	1034.607	-49.128
1200	772.738	1304.852	847.823	548.435	394.629	1092.816	-47.568
1300	790.255	1367.414	885.408	626.608	395.779	1150.956	-46.245
1400	805.214	1426.540	921.968	706.400	397.264	1208.999	-45.107
1500	818.062	1482.543	957.490	787.580	399.011	1266.927	-44.117
1600	829.156	1535.703	991.981	869.954	400.909	1324.725	-43.247
1700	838.784	1586.265	1025.464	953.363	402.891	1382.381	-42.475
1800	847.180	1634.452	1057.969	1037.670	404.892	1439.975	-41.786
1900	854.535	1680.458	1089.530	1122.764	406.886	1497.412	-41.166
2000	861.007	1724.458	1120.184	1208.548	408.824	1554.768	-40.606
2100	866.725	1766.608	1149.970	1294.940	410.638	1612.017	-40.096
2200	871.798	1807.047	1178.924	1381.871	412.329	1669.185	-39.631
2300	876.316	1845.902	1207.084	1469.281	413.890	1726.279	-39.204
2400	880.354	1883.285	1234.485	1557.119	415.260	1783.266	-38.811
2500	883.975	1919.297	1261.162	1645.338	416.449	1840.299	-38.450
2600	887.234	1954.032	1287.147	1733.901	417.427	1897.186	-38.114
2700	890.176	1987.572	1312.471	1822.774	418.196	1954.103	-37.804
2800	892.839	2019.995	1337.164	1911.927	418.734	2011.015	-37.515
2900	895.257	2051.369	1361.253	2001.334	419.014	2067.865	-37.246
3000	897.459	2081.757	1384.766	2090.972	419.077	2124.733	-36.994
3100	899.468	2111.218	1407.728	2180.819	418.853	2181.535	-36.758
3200	901.307	2139.804	1430.160	2270.859	418.379	2238.414	-36.538
3300	902.993	2167.565	1452.087	2361.076	417.639	2295.346	-36.332
3400	904.543	2194.545	1473.530	2451.454	416.609	2352.228	-36.137
3500	905.971	2220.787	1494.507	2541.980	415.292	2409.128	-35.954
3600	907.289	2246.327	1515.037	2632.644	413.709	2466.147	-35.782
3700	908.508	2271.203	1535.140	2723.435	411.832	2523.229	-35.621
3800	909.638	2295.447	1554.830	2814.343	409.637	2580.313	-35.468
3900	910.686	2319.089	1574.125	2905.360	407.161	2637.413	-35.323
4000	911.661	2342.158	1593.038	2996.478	404.389	2694.702	-35.188
4100	912.568	2364.680	1611.585	3087.690	401.290	2752.000	-35.060
4200	913.415	2386.681	1629.779	3178.989	397.888	2809.368	-34.939
4300	914.206	2408.184	1647.632	3270.371	394.172	2866.743	-34.823
4400	914.946	2429.209	1665.157	3361.829	390.149	2924.288	-34.715
4500	915.639	2449.779	1682.366	3453.358	385.832	2981.978	-34.613
4600	916.290	2469.911	1699.268	3544.955	381.174	3039.774	-34.517
4700	916.900	2489.623	1715.875	3636.615	376.190	3097.574	-34.425
4800	917.475	2508.933	1732.197	3728.334	370.920	3155.578	-34.339
4900	918.016	2527.856	1748.242	3820.109	365.299	3213.574	-34.256
5000	918.525	2546.408	1764.021	3911.936	359.409	3271.855	-34.180

3.219. Dibenz[*a,l*]aceanthrylene



Other names: Naphtho[1,2-*a*]fluoranthene
1',2'-Naphtho-1,2-fluoranthene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 203-07-6
Point Group: C₁

Length: 13.13 Å
Width: 11.03 Å
Breadth: 5.031 Å
L/B Ratio: 1.190

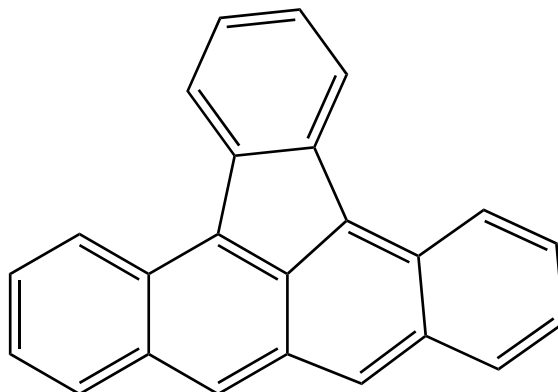
Cartesian coordinates:

C	-0.4315	2.5801	0.3913	C	-1.5257	-0.8879	-0.0733	H	0.6523	2.6927	0.5235
C	2.2318	1.3959	-0.6475	C	-1.4720	-2.2794	-0.0938	H	3.4905	3.0524	-1.1854
C	2.1392	0.0997	-0.1121	C	-0.1970	-2.8496	0.0759	H	4.2775	-2.4364	0.8283
C	0.8662	-0.5980	0.0319	C	-2.7651	-0.1711	-0.1379	H	2.1834	-3.7492	0.6553
C	-0.3998	-0.0171	0.0247	C	-3.9371	-0.8562	-0.2696	H	-0.0992	-3.9395	0.1495
C	-0.9850	1.3405	0.1278	C	-3.8871	-2.2800	-0.3242	H	-2.6982	-4.0703	-0.2651
C	3.3423	-0.5615	0.2054	C	-2.7106	-2.9755	-0.2333	H	-4.9005	-0.3399	-0.3281
C	4.5730	0.1120	0.1108	C	-1.2623	3.7026	0.4784	H	-4.8323	-2.8223	-0.4362
C	4.6254	1.4083	-0.3604	C	-2.6346	3.5960	0.3125	H	-4.3099	2.2525	-0.0288
C	3.4474	2.0412	-0.7674	C	-3.2249	2.3499	0.0791	H	-3.2647	4.4891	0.3747
C	0.9233	-2.0324	0.1673	C	-2.4083	1.2400	0.0024	H	-0.8143	4.6810	0.6819
C	2.1877	-2.6686	0.4676	H	5.5827	1.9340	-0.4338	H	1.3193	1.9073	-0.9832
C	3.3302	-1.9614	0.5485	H	5.4934	-0.4085	0.3999				

Table 3.219: Table of thermodynamic data as a function of temperature for Dibenz[*a,l*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.730	455.978	455.978	∞
100	98.194	332.880	718.997	-38.612	479.427	518.932	-271.057
200	192.914	428.366	549.845	-24.296	467.061	563.358	-147.131
250	248.427	477.326	530.421	-13.274	461.207	588.109	-122.876
298.15	302.818	525.741	525.741	0.000	455.978	613.037	-107.399
300	304.886	527.621	525.747	0.562	455.786	614.011	-106.907
350	359.313	578.747	529.661	17.180	450.957	640.774	-95.628
400	409.838	630.075	539.006	36.428	446.757	668.177	-87.253
450	455.622	681.039	551.961	58.085	443.115	696.077	-80.797
500	496.546	731.203	567.385	81.909	439.953	724.375	-75.673
600	565.161	828.048	602.830	135.131	434.800	781.770	-68.058
700	619.417	919.401	641.597	194.463	431.014	839.921	-62.674
800	662.935	1005.056	681.735	258.657	428.434	898.517	-58.666
900	698.409	1085.256	722.164	326.783	426.901	957.366	-55.563
1000	727.723	1160.405	762.271	398.134	426.273	1016.348	-53.087
1100	752.209	1230.947	801.704	472.167	426.376	1075.364	-51.064
1200	772.840	1297.307	840.267	548.448	427.087	1134.328	-49.375
1300	790.348	1359.878	877.854	626.631	428.247	1193.222	-47.943
1400	805.299	1419.010	914.416	706.432	429.741	1252.018	-46.712
1500	818.140	1475.019	949.939	787.620	431.497	1310.699	-45.642
1600	829.227	1528.183	984.432	870.002	433.402	1369.250	-44.700
1700	838.849	1578.750	1017.916	953.417	435.390	1427.657	-43.866
1800	847.239	1626.940	1050.423	1037.731	437.398	1486.002	-43.122
1900	854.589	1672.949	1081.986	1122.830	439.398	1544.190	-42.452
2000	861.056	1716.952	1112.642	1208.619	441.341	1602.297	-41.847
2100	866.771	1759.104	1142.430	1295.016	443.160	1660.297	-41.297
2200	871.840	1799.545	1171.386	1381.952	444.854	1718.215	-40.795
2300	876.355	1838.402	1199.547	1469.366	446.419	1776.059	-40.335
2400	880.390	1875.786	1226.950	1557.207	447.793	1833.796	-39.911
2500	884.009	1911.800	1253.628	1645.430	448.986	1891.579	-39.522
2600	887.265	1946.536	1279.614	1733.996	449.967	1949.215	-39.159
2700	890.205	1980.078	1304.940	1822.872	450.739	2006.882	-38.825
2800	892.866	2012.501	1329.634	1912.028	451.280	2064.544	-38.514
2900	895.283	2043.876	1353.725	2001.438	451.563	2122.143	-38.223
3000	897.483	2074.265	1377.239	2091.078	451.628	2179.760	-37.952
3100	899.491	2103.727	1400.202	2180.928	451.406	2237.311	-37.698
3200	901.328	2132.314	1422.636	2270.970	450.935	2294.939	-37.460
3300	903.013	2160.075	1444.564	2361.188	450.197	2352.620	-37.238
3400	904.562	2187.056	1466.007	2451.568	449.169	2410.251	-37.028
3500	905.989	2213.298	1486.985	2542.097	447.854	2467.900	-36.831
3600	907.306	2238.839	1507.516	2632.762	446.273	2525.668	-36.646
3700	908.524	2263.715	1527.620	2723.555	444.397	2583.499	-36.472
3800	909.653	2287.959	1547.311	2814.464	442.204	2641.331	-36.307
3900	910.701	2311.602	1566.606	2905.483	439.729	2699.180	-36.151
4000	911.675	2334.671	1585.521	2996.602	436.958	2757.218	-36.005
4100	912.582	2357.194	1604.068	3087.815	433.861	2815.264	-35.866
4200	913.428	2379.195	1622.263	3179.116	430.461	2873.381	-35.735
4300	914.218	2400.698	1640.117	3270.499	426.746	2931.504	-35.610
4400	914.958	2421.724	1657.643	3361.958	422.724	2989.798	-35.493
4500	915.650	2442.294	1674.852	3453.489	418.408	3048.236	-35.382
4600	916.300	2462.426	1691.755	3545.087	413.751	3106.781	-35.278
4700	916.911	2482.139	1708.362	3636.748	408.768	3165.330	-35.178
4800	917.485	2501.449	1724.685	3728.468	403.499	3224.082	-35.084
4900	918.025	2520.372	1740.731	3820.244	397.879	3282.827	-34.995
5000	918.534	2538.924	1756.510	3912.072	391.990	3341.856	-34.911

3.220. Indeno[1,2,3-*fg*]naphthacene



Other names: Dibenzo[*a,f*]fluoranthene
 5,6-(1,2-Phenylene)naphthacene
 5,6-*o*-Phenylenenaphthacene
 10,11-Phenylenenaphthacene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 203-11-2
Point Group: C_{2v}

Length: 14.08 Å
Width: 11.06 Å
Breadth: 3.886 Å
L/B Ratio: 1.273

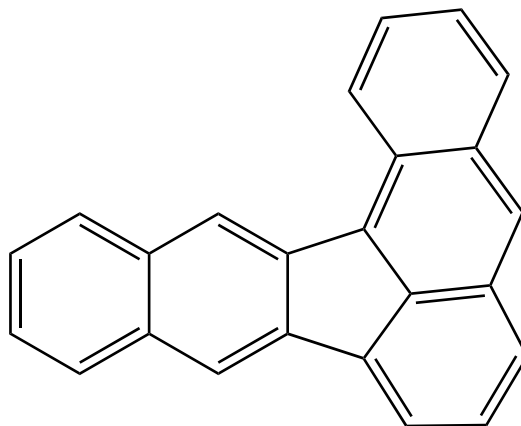
Cartesian coordinates:

C	-1.1434	3.0671	0.0000	C	-2.4239	-0.0428	0.0000	H	-4.0342	-3.0981	0.0000
C	-0.5538	1.8180	0.0000	C	-2.5761	-1.4746	0.0000	H	-3.4492	1.8767	0.0000
C	0.8722	1.6885	0.0000	C	-1.4829	-2.3357	0.0000	H	-1.6360	-3.4216	0.0000
C	1.6772	2.8110	0.0000	C	-3.9136	-2.0085	0.0000	H	0.9933	-3.6603	0.0000
C	1.0667	4.0697	0.0000	C	-4.9946	-1.1895	0.0000	H	3.4104	-3.7741	0.0000
C	-0.3162	4.1953	0.0000	C	-4.8348	0.2313	0.0000	H	5.6232	-2.6564	0.0000
C	1.2053	0.2596	0.0000	C	-3.5968	0.7850	0.0000	H	5.7930	-0.1877	0.0000
C	2.3765	-0.4788	0.0000	C	3.4877	-2.6806	0.0000	H	3.7310	1.2247	0.0000
C	2.2683	-1.9145	0.0000	C	4.6986	-2.0697	0.0000	H	2.7715	2.7032	0.0000
C	1.0379	-2.5647	0.0000	C	4.7974	-0.6434	0.0000	H	1.6928	4.9680	0.0000
C	-0.1656	-1.8239	0.0000	C	3.6793	0.1243	0.0000	H	-0.7703	5.1917	0.0000
C	-0.0389	-0.4284	0.0000	H	-5.7322	0.8586	0.0000	H	-2.2393	3.1582	0.0000
C	-1.1388	0.4725	0.0000	H	-6.0098	-1.5998	0.0000				

Table 3.220: Table of thermodynamic data as a function of temperature for Indeno[1,2,3-*fg*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.593	466.516	466.516	∞
100	101.530	335.493	726.993	-39.150	489.426	528.670	-276.143
200	195.611	433.092	555.757	-24.533	477.361	572.713	-149.574
250	250.835	482.623	536.156	-13.383	471.635	597.213	-124.778
298.15	304.961	531.440	531.440	0.000	466.516	621.876	-108.948
300	307.019	533.332	531.445	0.566	466.327	622.839	-108.444
350	361.182	584.767	535.384	17.284	461.598	649.309	-96.902
400	411.465	636.329	544.781	36.619	457.486	676.404	-88.328
450	457.033	687.471	557.800	58.352	453.920	703.987	-81.715
500	497.769	737.774	573.291	82.242	450.824	731.960	-76.466
600	566.078	834.814	608.864	135.570	445.777	788.687	-68.660
700	620.104	926.290	647.745	194.982	442.071	846.155	-63.140
800	663.448	1012.025	687.981	259.236	439.550	904.057	-59.028
900	698.791	1092.277	728.493	327.405	438.061	962.207	-55.844
1000	728.006	1167.461	768.671	398.790	437.466	1020.485	-53.304
1100	752.419	1238.026	808.166	472.847	437.594	1078.795	-51.227
1200	772.995	1304.403	846.781	549.146	438.323	1137.049	-49.493
1300	790.461	1366.983	884.412	627.342	439.496	1195.234	-48.024
1400	805.381	1426.123	921.013	707.154	441.000	1253.319	-46.761
1500	818.198	1482.137	956.571	788.349	442.763	1311.288	-45.662
1600	829.268	1535.304	991.095	870.735	444.672	1369.127	-44.696
1700	838.876	1585.873	1024.606	954.153	446.664	1426.821	-43.840
1800	847.256	1634.065	1057.137	1038.469	448.674	1484.455	-43.077
1900	854.599	1680.074	1088.722	1123.570	450.675	1541.930	-42.390
2000	861.060	1724.077	1119.397	1209.360	452.619	1599.324	-41.769
2100	866.771	1766.230	1149.202	1295.757	454.438	1656.612	-41.205
2200	871.837	1806.671	1178.174	1382.693	456.133	1713.818	-40.690
2300	876.349	1845.527	1206.351	1470.106	457.697	1770.949	-40.219
2400	880.382	1882.911	1233.767	1557.946	459.070	1827.973	-39.784
2500	884.000	1918.925	1260.457	1646.169	460.263	1885.044	-39.385
2600	887.255	1953.660	1286.455	1734.734	461.242	1941.968	-39.014
2700	890.194	1987.202	1311.791	1823.609	462.013	1998.922	-38.671
2800	892.855	2019.625	1336.495	1912.764	462.553	2055.871	-38.352
2900	895.271	2050.999	1360.595	2002.172	462.835	2112.758	-38.054
3000	897.471	2081.388	1384.117	2091.811	462.899	2169.663	-37.776
3100	899.479	2110.849	1407.088	2181.660	462.676	2226.502	-37.516
3200	901.317	2139.436	1429.529	2271.701	462.203	2283.417	-37.272
3300	903.002	2167.197	1451.464	2361.918	461.464	2340.386	-37.044
3400	904.551	2194.177	1472.914	2452.297	460.435	2397.305	-36.829
3500	905.978	2220.419	1493.898	2542.824	459.120	2454.242	-36.627
3600	907.296	2245.960	1514.435	2633.489	457.537	2511.298	-36.437
3700	908.514	2270.836	1534.544	2724.280	455.660	2568.417	-36.259
3800	909.643	2295.079	1554.240	2815.189	453.466	2625.537	-36.090
3900	910.691	2318.722	1573.540	2906.206	450.990	2682.674	-35.930
4000	911.665	2341.791	1592.459	2997.325	448.219	2740.000	-35.780
4100	912.572	2364.313	1611.012	3088.537	445.120	2797.334	-35.638
4200	913.419	2386.314	1629.210	3179.837	441.719	2854.739	-35.503
4300	914.209	2407.817	1647.068	3271.219	438.003	2912.150	-35.375
4400	914.949	2428.843	1664.598	3362.677	433.980	2969.732	-35.254
4500	915.642	2449.412	1681.810	3454.207	429.663	3027.459	-35.141
4600	916.292	2469.544	1698.717	3545.804	425.006	3085.292	-35.034
4700	916.903	2489.257	1715.328	3637.464	420.022	3143.129	-34.931
4800	917.477	2508.567	1731.653	3729.183	414.753	3201.169	-34.835
4900	918.018	2527.490	1747.703	3820.958	409.132	3259.202	-34.743
5000	918.527	2546.042	1763.484	3912.786	403.242	3317.519	-34.657

3.221. Naphth[2,3-*a*]aceanthrylene



Other names: Dibenzo[*a,k*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 84030-79-5

Point Group: C_s

Length: 14.38 Å

Width: 11.51 Å

Breadth: 3.890 Å

L/B Ratio: 1.249

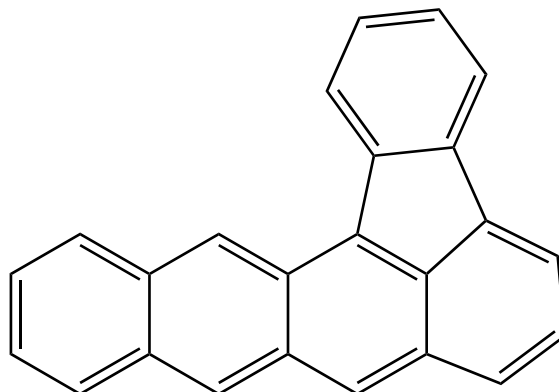
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C	1.8085	1.2855	0.0000	C	-0.5833	0.1557	0.0000	H	-3.6551	2.7807	0.0000
C	3.1993	0.9437	0.0000	C	-1.5385	1.1261	0.0000	H	-2.5420	-2.6932	0.0000
C	4.1568	2.0125	0.0000	C	-2.9137	0.7400	0.0000	H	-1.2600	2.1909	0.0000
C	3.7555	3.3116	0.0000	C	-3.2692	-0.6267	0.0000	H	-0.1893	-4.1384	0.0000
C	2.3699	3.6439	0.0000	C	-2.2562	-1.6356	0.0000	H	2.1943	-4.8234	0.0000
C	3.6387	-0.3883	0.0000	C	-0.9509	-1.2515	0.0000	H	4.0354	-3.1722	0.0000
C	2.7125	-1.4382	0.0000	C	-4.6410	-0.9850	0.0000	H	4.7126	-0.6097	0.0000
C	1.3593	-1.0827	0.0000	C	-5.6116	-0.0165	0.0000	H	5.2224	1.7552	0.0000
C	0.8826	0.2424	0.0000	C	-5.2564	1.3491	0.0000	H	4.4897	4.1240	0.0000
C	2.9902	-2.8447	0.0000	C	-3.9369	1.7217	0.0000	H	2.0819	4.7002	0.0000
C	1.9678	-3.7514	0.0000	H	-6.0470	2.1065	0.0000	H	0.3509	2.8994	0.0000
C	0.5879	-3.3680	0.0000	H	-6.6712	-0.2926	0.0000				

Table 3.221: Table of thermodynamic data as a function of temperature for Naphth[2,3-*a*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.868	434.885	434.885	∞
100	98.661	334.875	721.964	-38.709	458.236	497.542	-259.884
200	193.434	430.713	552.423	-24.342	445.920	541.748	-141.487
250	248.906	479.786	532.964	-13.295	440.092	566.379	-118.336
298.15	303.195	528.278	528.278	0.000	434.885	591.187	-103.571
300	305.258	530.160	528.284	0.563	434.692	592.156	-103.101
350	359.536	581.332	532.201	17.196	429.879	618.791	-92.348
400	409.910	632.680	541.553	36.451	425.686	646.064	-84.366
450	455.565	683.644	554.515	58.108	422.045	673.834	-78.215
500	496.392	733.797	569.944	81.927	418.877	702.002	-73.336
600	564.897	830.603	605.392	135.127	413.702	759.139	-66.088
700	619.124	921.913	644.155	194.431	409.888	817.037	-60.967
800	662.654	1007.529	684.284	258.596	407.279	875.383	-57.155
900	698.156	1087.697	724.703	326.695	405.719	933.987	-54.206
1000	727.503	1162.821	764.798	398.023	405.067	992.726	-51.854
1100	752.021	1233.343	804.221	472.035	405.150	1051.502	-49.931
1200	772.680	1299.689	842.773	548.298	405.844	1110.226	-48.326
1300	790.212	1362.247	880.350	626.467	406.989	1168.884	-46.965
1400	805.183	1421.370	916.902	706.256	408.470	1227.443	-45.796
1500	818.040	1477.372	952.417	787.433	410.215	1285.889	-44.778
1600	829.142	1530.530	986.902	869.805	412.111	1344.204	-43.883
1700	838.775	1581.092	1020.379	953.212	414.092	1402.376	-43.089
1800	847.175	1629.278	1052.879	1037.519	416.093	1460.488	-42.381
1900	854.533	1675.284	1084.435	1122.612	418.086	1518.442	-41.744
2000	861.007	1719.284	1115.086	1208.396	420.024	1576.316	-41.168
2100	866.727	1761.434	1144.868	1294.789	421.838	1634.082	-40.645
2200	871.801	1801.873	1173.819	1381.720	423.529	1691.768	-40.167
2300	876.320	1840.728	1201.976	1469.131	425.090	1749.379	-39.729
2400	880.359	1878.111	1229.374	1556.968	426.461	1806.883	-39.325
2500	883.981	1914.124	1256.048	1645.188	427.651	1864.434	-38.954
2600	887.240	1948.859	1282.031	1733.752	428.629	1921.838	-38.609
2700	890.182	1982.399	1307.353	1822.626	429.398	1979.273	-38.291
2800	892.845	2014.822	1332.044	1911.779	429.937	2036.702	-37.994
2900	895.263	2046.196	1356.132	2001.187	430.218	2094.069	-37.717
3000	897.465	2076.585	1379.643	2090.825	430.281	2151.454	-37.459
3100	899.474	2106.046	1402.603	2180.673	430.058	2208.774	-37.217
3200	901.313	2134.632	1425.034	2270.714	429.585	2266.169	-36.991
3300	902.999	2162.393	1446.960	2360.931	428.845	2323.618	-36.779
3400	904.549	2189.374	1468.401	2451.309	427.816	2381.018	-36.579
3500	905.977	2215.615	1489.376	2541.837	426.500	2438.435	-36.391
3600	907.295	2241.156	1509.906	2632.501	424.918	2495.971	-36.215
3700	908.514	2266.032	1530.007	2723.292	423.041	2553.571	-36.049
3800	909.643	2290.276	1549.697	2814.201	420.846	2611.171	-35.892
3900	910.691	2313.918	1568.990	2905.218	418.371	2668.788	-35.744
4000	911.666	2336.987	1587.903	2996.337	415.599	2726.595	-35.605
4100	912.573	2359.510	1606.449	3087.549	412.501	2784.409	-35.473
4200	913.420	2381.511	1624.642	3178.849	409.100	2842.295	-35.348
4300	914.211	2403.013	1642.494	3270.231	405.384	2900.186	-35.230
4400	914.951	2424.039	1660.019	3361.690	401.361	2958.249	-35.118
4500	915.644	2444.609	1677.226	3453.220	397.044	3016.456	-35.013
4600	916.294	2464.741	1694.128	3544.817	392.388	3074.769	-34.914
4700	916.905	2484.453	1710.735	3636.477	387.404	3133.086	-34.820
4800	917.479	2503.763	1727.056	3728.197	382.134	3191.606	-34.731
4900	918.019	2522.687	1743.101	3819.972	376.513	3250.120	-34.646
5000	918.529	2541.238	1758.878	3911.800	370.624	3308.917	-34.567

3.222. Indeno[1,2,3-*de*]naphthacene



Other names: Naphtho[2,3-*a*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 314-51-2

Point Group: C_s

Length: 14.32 Å

Width: 11.02 Å

Breadth: 3.893 Å

L/B Ratio: 1.299

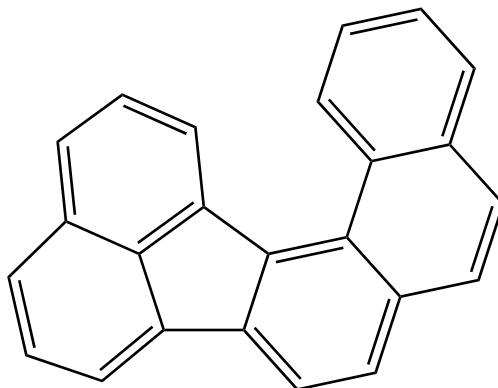
Cartesian coordinates:

C	-1.7444	0.6931	0.0000	C	-0.2325	2.5312	0.0000	H	4.7713	2.7570	0.0000
C	-0.7201	-0.2570	0.0000	C	-1.5467	2.0853	0.0000	H	3.9538	-2.1803	0.0000
C	-3.0506	0.0736	0.0000	C	-2.7443	2.8834	0.0000	H	2.3564	3.1583	0.0000
C	5.4070	-0.6095	0.0000	C	-3.9715	2.2907	0.0000	H	1.5175	-1.7808	0.0000
C	5.6404	0.8022	0.0000	C	-4.1530	0.8644	0.0000	H	-0.0155	3.6060	0.0000
C	4.6023	1.6742	0.0000	C	-1.3734	-1.5723	0.0000	H	-2.6426	3.9740	0.0000
C	4.1434	-1.1009	0.0000	C	-2.7913	-1.3716	0.0000	H	-4.8745	2.9114	0.0000
C	3.0112	-0.2128	0.0000	C	-3.6533	-2.4491	0.0000	H	-5.1658	0.4496	0.0000
C	3.2438	1.1984	0.0000	C	-3.1058	-3.7379	0.0000	H	-4.7376	-2.3001	0.0000
C	2.1739	2.0761	0.0000	C	-1.7317	-3.9339	0.0000	H	-3.7765	-4.6035	0.0000
C	1.7146	-0.6959	0.0000	C	-0.8477	-2.8494	0.0000	H	-1.3289	-4.9521	0.0000
C	0.6161	0.1878	0.0000	H	6.2720	-1.2809	0.0000	H	0.2421	-2.9962	0.0000
C	0.8410	1.6046	0.0000	H	6.6754	1.1594	0.0000				

Table 3.222: Table of thermodynamic data as a function of temperature for Indeno[1,2,3-*de*]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-45.226	460.590	460.590	∞
100	99.926	338.655	727.890	-38.924	483.726	522.655	-273.001
200	194.479	435.270	557.499	-24.446	471.522	566.439	-147.936
250	249.962	484.577	537.961	-13.346	465.746	590.836	-123.446
298.15	304.269	533.257	533.257	0.000	460.590	615.408	-107.815
300	306.332	535.145	533.263	0.565	460.400	616.368	-107.317
350	360.618	586.484	537.193	17.252	455.640	642.749	-95.923
400	410.983	637.976	546.574	36.561	451.502	669.761	-87.460
450	456.613	689.065	559.574	58.271	447.913	697.263	-80.934
500	497.401	739.327	575.045	82.141	444.797	725.157	-75.755
600	565.808	836.308	610.579	135.437	439.718	781.732	-68.054
700	619.928	927.750	649.426	194.827	435.990	839.052	-62.610
800	663.357	1013.467	689.633	259.068	433.456	896.810	-58.554
900	698.769	1093.712	730.121	327.232	431.962	954.816	-55.415
1000	728.038	1168.897	770.280	398.617	431.367	1012.950	-52.910
1100	752.491	1239.467	809.759	472.679	431.500	1071.116	-50.862
1200	773.094	1305.851	848.362	548.987	432.238	1129.226	-49.153
1300	790.578	1368.441	885.984	627.194	433.422	1187.265	-47.704
1400	805.509	1427.590	922.577	707.018	434.938	1245.204	-46.458
1500	818.332	1483.612	958.128	788.226	436.714	1303.027	-45.374
1600	829.404	1536.788	992.647	870.626	438.637	1360.717	-44.422
1700	839.011	1587.366	1026.155	954.058	440.643	1418.263	-43.577
1800	847.389	1635.565	1058.683	1038.387	442.666	1475.746	-42.824
1900	854.728	1681.582	1090.265	1123.501	444.680	1533.071	-42.146
2000	861.185	1725.591	1120.939	1209.304	446.637	1590.315	-41.534
2100	866.890	1767.749	1150.743	1295.713	448.468	1647.450	-40.977
2200	871.952	1808.196	1179.714	1382.660	450.174	1704.504	-40.469
2300	876.459	1847.057	1207.890	1470.085	451.750	1761.482	-40.004
2400	880.487	1884.446	1235.306	1557.936	453.134	1818.353	-39.575
2500	884.100	1920.463	1261.996	1646.169	454.337	1875.270	-39.181
2600	887.350	1955.203	1287.994	1734.744	455.326	1932.040	-38.814
2700	890.285	1988.748	1313.330	1823.628	456.106	1988.840	-38.476
2800	892.941	2021.174	1338.034	1912.792	456.655	2045.635	-38.161
2900	895.354	2052.551	1362.135	2002.208	456.945	2102.367	-37.867
3000	897.549	2082.943	1385.658	2091.855	457.017	2159.116	-37.593
3100	899.554	2112.406	1408.628	2181.712	456.802	2215.799	-37.335
3200	901.388	2140.996	1431.070	2271.760	456.336	2272.559	-37.095
3300	903.070	2168.759	1453.006	2361.984	455.604	2329.371	-36.870
3400	904.616	2195.741	1474.456	2452.370	454.582	2386.134	-36.658
3500	906.040	2221.985	1495.441	2542.903	453.272	2442.914	-36.458
3600	907.355	2247.527	1515.979	2633.574	451.696	2499.814	-36.271
3700	908.570	2272.405	1536.088	2724.371	449.825	2556.776	-36.094
3800	909.697	2296.650	1555.785	2815.285	447.636	2613.739	-35.928
3900	910.742	2320.293	1575.086	2906.308	445.166	2670.718	-35.770
4000	911.714	2343.364	1594.006	2997.431	442.399	2727.888	-35.622
4100	912.620	2365.888	1612.559	3088.648	439.305	2785.064	-35.481
4200	913.464	2387.890	1630.758	3179.953	435.909	2842.312	-35.349
4300	914.253	2409.393	1648.617	3271.339	432.197	2899.565	-35.222
4400	914.991	2430.420	1666.147	3362.802	428.179	2956.990	-35.103
4500	915.682	2450.991	1683.360	3454.336	423.866	3014.558	-34.991
4600	916.331	2471.123	1700.268	3545.937	419.213	3072.233	-34.886
4700	916.940	2490.837	1716.879	3637.601	414.233	3129.912	-34.784
4800	917.513	2510.148	1733.205	3729.324	408.967	3187.794	-34.690
4900	918.052	2529.072	1749.255	3821.102	403.349	3245.669	-34.599
5000	918.561	2547.624	1765.037	3912.933	397.463	3303.828	-34.514

3.223. Naphtho[1,2-j]fluoranthene



Formula: $C_{24}H_{14}$
Mass: 302.368 g/mol
CAS Number: 908069-85-2
Point Group: C_1

Length: 13.68 Å
Width: 10.25 Å
Breadth: 5.083 Å
L/B Ratio: 1.335

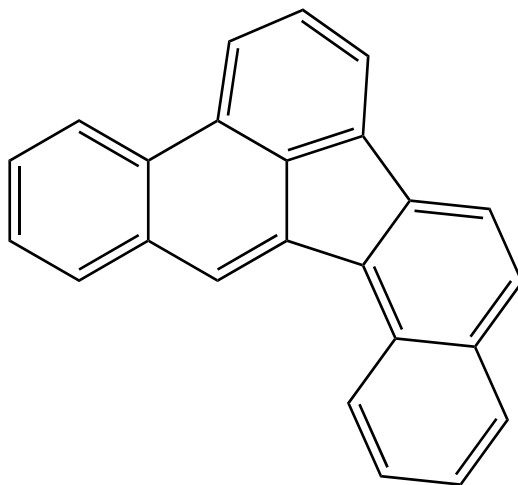
Cartesian coordinates:

C	-4.6063	0.9508	-0.1281	C	1.9439	2.9401	-0.5544	H	1.7513	3.9939	-0.7852
C	-3.5881	-0.0221	-0.1941	C	2.4518	-1.0908	0.1929	H	5.6644	1.1181	-0.0203
C	-2.2564	0.3148	0.1228	C	1.0651	-1.5638	0.1612	H	5.8133	-1.3206	0.3746
C	-2.0182	1.6055	0.6349	C	0.6228	-2.8812	0.1849	H	3.7886	-2.7564	0.4770
C	-3.0265	2.5406	0.7296	C	-0.7256	-3.1138	-0.0001	H	1.3348	-3.7033	0.3097
C	-4.3275	2.2234	0.3179	C	-1.6306	-2.0435	-0.1182	H	-1.1015	-4.1422	-0.0572
C	-1.2124	-0.6915	0.0063	C	-3.0053	-2.3546	-0.4118	H	-3.2714	-3.4052	-0.5786
C	0.1781	-0.4586	0.0262	C	-3.9344	-1.3802	-0.5103	H	-4.9708	-1.6060	-0.7857
C	1.0164	0.7531	-0.1351	C	3.6799	-1.6778	0.3262	H	-5.6265	0.6768	-0.4209
C	0.8213	2.0750	-0.4380	C	4.8322	-0.8473	0.2573	H	-5.1166	2.9802	0.3707
C	2.3748	0.3179	-0.0052	C	4.7569	0.5081	0.0414	H	-2.8141	3.5368	1.1315
C	3.4906	1.1388	-0.1119	H	4.0801	3.2042	-0.4771	H	-0.1866	2.4865	-0.5784
C	3.2373	2.5106	-0.3891	H	-1.0088	1.8719	0.9754				

Table 3.223: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*j*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.587	450.619	450.619	∞
100	97.479	332.733	717.671	-38.494	474.185	513.706	-268.327
200	192.311	427.702	548.961	-24.252	461.745	558.175	-145.777
250	247.990	476.547	529.568	-13.255	455.866	582.963	-121.801
298.15	302.483	524.895	524.895	0.000	450.619	607.930	-106.505
300	304.554	526.772	524.901	0.562	450.426	608.905	-106.018
350	359.044	577.853	528.810	17.165	445.582	635.713	-94.873
400	409.609	629.147	538.147	36.400	441.370	663.161	-86.598
450	455.423	680.085	551.094	58.046	437.717	691.108	-80.220
500	496.371	730.230	566.508	81.861	434.546	719.454	-75.159
600	565.023	827.047	601.935	135.067	429.377	776.948	-67.638
700	619.308	918.381	640.685	194.387	425.579	835.200	-62.322
800	662.848	1004.023	680.808	258.572	422.989	893.898	-58.364
900	698.338	1084.213	721.225	326.689	421.448	952.852	-55.301
1000	727.664	1159.356	761.321	398.034	420.814	1011.938	-52.857
1100	752.161	1229.892	800.745	472.062	420.912	1071.060	-50.859
1200	772.800	1296.249	839.300	548.338	421.618	1130.129	-49.192
1300	790.313	1358.816	876.880	626.517	422.774	1189.130	-47.779
1400	805.269	1417.946	913.435	706.316	424.265	1248.032	-46.564
1500	818.114	1473.953	948.952	787.501	426.018	1306.819	-45.507
1600	829.204	1527.116	983.440	869.880	427.920	1365.476	-44.577
1700	838.829	1577.681	1016.921	953.293	429.907	1423.990	-43.753
1800	847.221	1625.870	1049.423	1037.605	431.913	1482.443	-43.018
1900	854.573	1671.879	1080.982	1122.703	433.911	1540.737	-42.357
2000	861.042	1715.880	1111.635	1208.490	435.852	1598.951	-41.759
2100	866.758	1758.032	1141.420	1294.886	437.670	1657.058	-41.216
2200	871.829	1798.473	1170.373	1381.820	439.363	1715.084	-40.720
2300	876.344	1837.329	1198.532	1469.233	440.927	1773.035	-40.266
2400	880.380	1874.712	1225.932	1557.073	442.300	1830.879	-39.847
2500	884.000	1910.726	1252.608	1645.295	443.492	1888.770	-39.463
2600	887.257	1945.462	1278.592	1733.861	444.472	1946.514	-39.105
2700	890.197	1979.003	1303.916	1822.736	445.243	2004.288	-38.774
2800	892.859	2011.426	1328.608	1911.891	445.783	2062.057	-38.467
2900	895.276	2042.801	1352.697	2001.300	446.066	2119.764	-38.180
3000	897.477	2073.190	1376.210	2090.939	446.130	2177.488	-37.913
3100	899.485	2102.651	1399.171	2180.789	445.908	2235.147	-37.661
3200	901.323	2131.238	1421.603	2270.830	445.435	2292.882	-37.427
3300	903.008	2158.999	1443.530	2361.048	444.697	2350.671	-37.207
3400	904.558	2185.980	1464.972	2451.428	443.669	2408.409	-37.000
3500	905.985	2212.222	1485.949	2541.956	442.354	2466.166	-36.805
3600	907.302	2237.763	1506.479	2632.621	440.772	2524.042	-36.622
3700	908.520	2262.639	1526.581	2723.413	438.896	2581.980	-36.450
3800	909.649	2286.883	1546.272	2814.322	436.702	2639.920	-36.287
3900	910.697	2310.525	1565.566	2905.340	434.227	2697.876	-36.133
4000	911.671	2333.594	1584.480	2996.459	431.456	2756.023	-35.989
4100	912.579	2356.117	1603.026	3087.672	428.358	2814.176	-35.852
4200	913.425	2378.118	1621.220	3178.973	424.958	2872.401	-35.723
4300	914.215	2399.621	1639.073	3270.355	421.242	2930.631	-35.599
4400	914.955	2420.647	1656.598	3361.814	417.220	2989.033	-35.484
4500	915.648	2441.217	1673.807	3453.345	412.904	3047.579	-35.375
4600	916.298	2461.349	1690.709	3544.942	408.247	3106.232	-35.272
4700	916.908	2481.061	1707.316	3636.603	403.264	3164.888	-35.173
4800	917.482	2500.371	1723.638	3728.323	397.995	3223.748	-35.081
4900	918.023	2519.295	1739.683	3820.098	392.374	3282.600	-34.992
5000	918.532	2537.847	1755.461	3911.926	386.485	3341.737	-34.910

3.224. Naphth[2,1-*e*]acephenanthrylene



Other names: Dibenzo[*b,l*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

Point Group: C_s

Length: 14.38 Å

Width: 10.53 Å

Breadth: 3.889 Å

L/B Ratio: 1.365

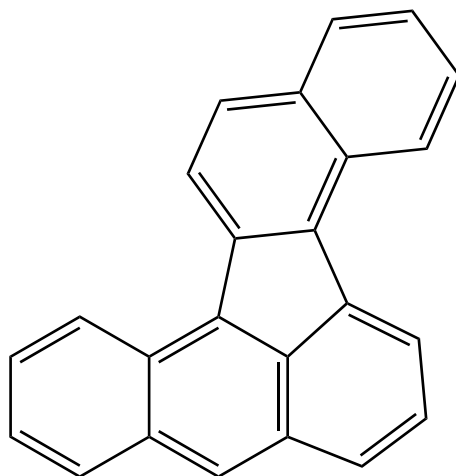
Cartesian coordinates:

C	4.3557	-2.5828	0.0000	C	-0.0364	2.0957	0.0000	H	4.9007	0.7885	0.0000
C	5.0563	-1.3669	0.0000	C	-1.3051	0.1239	0.0000	H	2.4333	-3.5433	0.0000
C	4.3691	-0.1731	0.0000	C	-1.3924	1.5298	0.0000	H	0.2870	-2.3981	0.0000
C	2.9781	-2.5921	0.0000	C	-2.6333	2.1814	0.0000	H	3.8463	2.5254	0.0000
C	2.2502	-1.3830	0.0000	C	-3.7793	1.4207	0.0000	H	2.3357	4.4975	0.0000
C	2.9611	-0.1598	0.0000	C	-2.4734	-0.6665	0.0000	H	-0.1373	4.2510	0.0000
C	0.8051	-1.4271	0.0000	C	-3.7220	0.0032	0.0000	H	-2.6735	3.2755	0.0000
C	2.2266	1.0862	0.0000	C	-4.9172	-0.7712	0.0000	H	-4.7620	1.9064	0.0000
C	2.7557	2.3980	0.0000	C	-4.8600	-2.1366	0.0000	H	-5.8819	-0.2511	0.0000
C	1.9079	3.4889	0.0000	C	-3.6101	-2.8034	0.0000	H	-5.7787	-2.7324	0.0000
C	0.4993	3.3608	0.0000	C	-2.4454	-2.0893	0.0000	H	-3.5924	-3.8981	0.0000
C	0.1140	-0.2616	0.0000	H	4.9129	-3.5254	0.0000	H	-1.4663	-2.5929	0.0000
C	0.8472	0.9827	0.0000	H	6.1511	-1.3739	0.0000				

Table 3.224: Table of thermodynamic data as a function of temperature for Naphth[2,1-*e*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.940	416.727	416.727	∞
100	99.505	336.308	723.343	-38.704	440.083	479.246	-250.327
200	193.303	432.422	553.935	-24.303	427.802	523.288	-136.666
250	248.474	481.431	534.510	-13.270	421.959	547.835	-114.462
298.15	302.627	529.833	529.833	0.000	416.727	572.566	-100.309
300	304.687	531.711	529.839	0.562	416.533	573.531	-99.859
350	358.944	582.793	533.749	17.166	411.690	600.092	-89.557
400	409.359	634.064	543.085	36.392	407.469	627.293	-81.914
450	455.079	684.967	556.027	58.023	403.801	654.996	-76.028
500	495.974	735.072	571.435	81.819	400.611	683.099	-71.361
600	564.593	831.812	606.840	134.983	395.401	740.112	-64.431
700	618.892	923.081	645.566	194.260	391.560	797.891	-59.538
800	662.465	1008.670	685.663	258.405	388.930	856.122	-55.898
900	697.992	1088.817	726.054	326.486	387.353	914.613	-53.082
1000	727.355	1163.925	766.126	397.799	386.685	973.241	-50.836
1100	751.885	1234.433	805.528	471.796	386.754	1031.907	-49.000
1200	772.553	1300.767	844.061	548.047	387.435	1090.523	-47.468
1300	790.093	1363.316	881.621	626.203	388.568	1149.073	-46.169
1400	805.071	1422.431	918.159	705.980	390.037	1207.526	-45.052
1500	817.935	1478.424	953.660	787.147	391.771	1265.866	-44.080
1600	829.043	1531.576	988.133	869.509	393.657	1324.076	-43.226
1700	838.683	1582.132	1021.599	952.907	395.628	1382.144	-42.467
1800	847.088	1630.313	1054.089	1037.204	397.620	1440.152	-41.791
1900	854.452	1676.315	1085.636	1122.289	399.605	1498.003	-41.182
2000	860.931	1720.311	1116.278	1208.065	401.535	1555.774	-40.632
2100	866.656	1762.457	1146.052	1294.451	403.342	1613.438	-40.131
2200	871.734	1802.893	1174.996	1381.375	405.026	1671.022	-39.674
2300	876.257	1841.745	1203.146	1468.779	406.581	1728.530	-39.255
2400	880.300	1879.125	1230.538	1556.610	407.945	1785.933	-38.869
2500	883.925	1915.136	1257.206	1644.825	409.130	1843.383	-38.515
2600	887.187	1949.869	1283.183	1733.383	410.102	1900.686	-38.184
2700	890.132	1983.407	1308.499	1822.252	410.866	1958.019	-37.879
2800	892.798	2015.828	1333.185	1911.401	411.400	2015.348	-37.596
2900	895.219	2047.201	1357.269	2000.803	411.677	2072.615	-37.331
3000	897.423	2077.588	1380.775	2090.437	411.736	2129.899	-37.084
3100	899.435	2107.047	1403.731	2180.282	411.508	2187.118	-36.852
3200	901.275	2135.633	1426.158	2270.318	411.031	2244.414	-36.636
3300	902.964	2163.393	1448.080	2360.532	410.288	2301.763	-36.433
3400	904.515	2190.372	1469.517	2450.907	409.255	2359.062	-36.242
3500	905.945	2216.613	1490.490	2541.431	407.936	2416.380	-36.062
3600	907.264	2242.153	1511.016	2632.092	406.351	2473.816	-35.893
3700	908.484	2267.028	1531.114	2722.880	404.471	2531.316	-35.735
3800	909.615	2291.271	1550.801	2813.786	402.273	2588.817	-35.585
3900	910.665	2314.912	1570.092	2904.800	399.795	2646.335	-35.443
4000	911.640	2337.981	1589.002	2995.916	397.021	2704.042	-35.310
4100	912.549	2360.503	1607.545	3087.126	393.920	2761.757	-35.184
4200	913.397	2382.503	1625.736	3178.424	390.517	2819.544	-35.065
4300	914.188	2404.005	1643.586	3269.804	386.798	2877.336	-34.952
4400	914.929	2425.031	1661.108	3361.260	382.774	2935.299	-34.846
4500	915.623	2445.600	1678.313	3452.788	378.455	2993.407	-34.746
4600	916.274	2465.731	1695.213	3544.383	373.796	3051.621	-34.652
4700	916.886	2485.443	1711.817	3636.041	368.810	3109.839	-34.561
4800	917.461	2504.753	1728.137	3727.759	363.539	3168.260	-34.477
4900	918.002	2523.676	1744.180	3819.532	357.916	3226.675	-34.396
5000	918.512	2542.227	1759.956	3911.358	352.025	3285.373	-34.321

3.225. Naphth[2,1-*a*]aceanthrylene



Other names: Dibenzo[*a,j*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 75519-75-4

Point Group: C_s

Length: 14.88 Å

Width: 10.80 Å

Breadth: 3.885 Å

L/B Ratio: 1.378

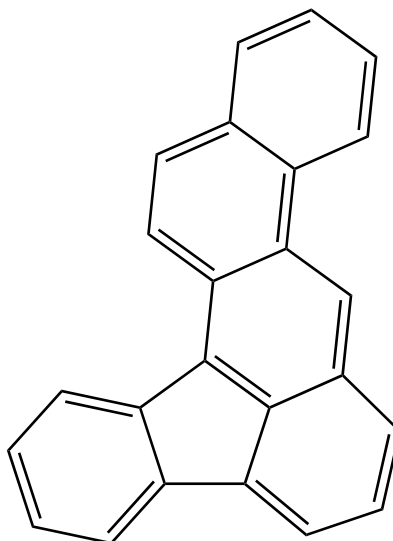
Cartesian coordinates:

C	-4.4056	-1.9106	0.0000	C	1.3571	3.4554	0.0000	H	5.5427	0.5162	0.0000
C	-3.0256	-1.5603	0.0000	C	0.0214	3.7475	0.0000	H	1.8405	-2.8500	0.0000
C	-2.6687	-0.1894	0.0000	C	-0.9944	2.7390	0.0000	H	3.9528	2.3355	0.0000
C	-3.6926	0.7987	0.0000	C	3.1199	1.6223	0.0000	H	2.1090	4.2519	0.0000
C	-5.0081	0.4296	0.0000	C	3.3800	0.2432	0.0000	H	-0.3049	4.7934	0.0000
C	-5.3683	-0.9403	0.0000	C	2.3297	-0.7311	0.0000	H	-2.0578	3.0190	0.0000
C	-1.2954	0.1311	0.0000	C	1.0137	-0.2680	0.0000	H	-2.3337	-3.6163	0.0000
C	-0.3193	-0.8862	0.0000	C	4.7359	-0.2261	0.0000	H	0.0976	-3.0097	0.0000
C	-0.6877	-2.2398	0.0000	C	5.0164	-1.5566	0.0000	H	-3.3948	1.8590	0.0000
C	-2.0232	-2.5651	0.0000	C	3.9666	-2.5197	0.0000	H	-5.7990	1.1867	0.0000
C	-0.6134	1.4321	0.0000	C	2.6663	-2.1216	0.0000	H	-6.4297	-1.2093	0.0000
C	0.7931	1.1235	0.0000	H	4.2277	-3.5830	0.0000	H	-4.6801	-2.9716	0.0000
C	1.8011	2.0921	0.0000	H	6.0527	-1.9102	0.0000				

Table 3.225: Table of thermodynamic data as a function of temperature for Naphth[2,1-*a*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.189	449.851	449.851	∞
100	99.887	339.044	727.700	-38.866	473.045	511.934	-267.402
200	194.196	435.547	557.574	-24.405	460.823	555.684	-145.127
250	249.547	484.776	538.068	-13.323	455.030	580.070	-121.196
298.15	303.737	533.373	533.373	0.000	449.851	604.635	-105.927
300	305.797	535.258	533.378	0.564	449.660	605.594	-105.441
350	360.005	586.508	537.302	17.222	444.871	631.972	-94.315
400	410.334	637.915	546.667	36.499	440.701	658.984	-86.053
450	455.956	688.927	559.646	58.177	437.079	686.491	-79.684
500	496.754	739.120	575.092	82.014	433.931	714.394	-74.631
600	565.195	835.986	610.574	135.247	428.789	770.996	-67.120
700	619.349	927.336	649.369	194.577	425.001	828.353	-61.811
800	662.806	1012.978	689.526	258.762	422.410	886.156	-57.859
900	698.244	1093.160	729.968	326.872	420.863	944.214	-54.800
1000	727.539	1168.291	770.084	398.206	420.217	1002.406	-52.359
1100	752.016	1238.815	809.524	472.220	420.301	1060.635	-50.364
1200	772.646	1305.158	848.090	548.482	420.993	1118.813	-48.700
1300	790.156	1367.713	885.678	626.645	422.134	1176.923	-47.288
1400	805.113	1426.831	922.240	706.428	423.609	1234.936	-46.075
1500	817.961	1482.828	957.763	787.598	425.346	1292.836	-45.020
1600	829.057	1535.980	992.254	869.962	427.233	1350.606	-44.092
1700	838.688	1586.537	1025.737	953.360	429.206	1408.234	-43.269
1800	847.087	1634.719	1058.242	1037.658	431.198	1465.801	-42.536
1900	854.446	1680.720	1089.802	1122.743	433.183	1523.211	-41.875
2000	860.921	1724.715	1120.456	1208.518	435.112	1580.542	-41.279
2100	866.644	1766.861	1150.241	1294.902	436.918	1637.765	-40.736
2200	871.721	1807.297	1179.194	1381.825	438.600	1694.909	-40.241
2300	876.242	1846.148	1207.353	1469.228	440.153	1751.977	-39.788
2400	880.284	1883.527	1234.753	1557.058	441.516	1808.940	-39.370
2500	883.909	1919.537	1261.429	1645.270	442.699	1865.949	-38.986
2600	887.171	1954.269	1287.413	1733.827	443.670	1922.812	-38.629
2700	890.116	1987.808	1312.736	1822.694	444.433	1979.705	-38.299
2800	892.782	2020.228	1337.427	1911.841	444.965	2036.594	-37.992
2900	895.203	2051.600	1361.516	2001.242	445.240	2093.421	-37.706
3000	897.408	2081.986	1385.028	2090.875	445.297	2150.266	-37.439
3100	899.420	2111.445	1407.988	2180.718	445.068	2207.045	-37.188
3200	901.261	2140.030	1430.420	2270.753	444.590	2263.901	-36.954
3300	902.949	2167.790	1452.346	2360.965	443.845	2320.810	-36.735
3400	904.501	2194.769	1473.787	2451.338	442.811	2377.670	-36.528
3500	905.931	2221.009	1494.763	2541.861	441.491	2434.548	-36.333
3600	907.251	2246.549	1515.293	2632.521	439.904	2491.545	-36.151
3700	908.472	2271.423	1535.394	2723.308	438.022	2548.605	-35.979
3800	909.603	2295.666	1555.084	2814.212	435.824	2605.666	-35.817
3900	910.653	2319.307	1574.377	2905.226	433.344	2662.744	-35.663
4000	911.629	2342.375	1593.290	2996.340	430.569	2720.012	-35.519
4100	912.538	2364.897	1611.836	3087.549	427.467	2777.288	-35.382
4200	913.386	2386.897	1630.029	3178.846	424.062	2834.635	-35.253
4300	914.178	2408.399	1647.882	3270.224	420.343	2891.987	-35.130
4400	914.919	2429.424	1665.406	3361.680	416.317	2949.511	-35.014
4500	915.613	2449.993	1682.614	3453.207	411.997	3007.180	-34.906
4600	916.265	2470.124	1699.515	3544.801	407.338	3064.955	-34.803
4700	916.876	2489.836	1716.122	3636.458	402.351	3122.734	-34.705
4800	917.452	2509.146	1732.443	3728.175	397.079	3180.716	-34.613
4900	917.993	2528.068	1748.487	3819.947	391.455	3238.691	-34.524
5000	918.504	2546.620	1764.265	3911.773	385.563	3296.950	-34.442

3.226. Dibenz[*a,j*]aceanthrylene



Other names: 15,16-Benzodehydrocholanthrene
Naphtho[2,1-*a*]fluoranthene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 203-20-3
Point Group: C_s

Length: 14.91 Å
Width: 10.79 Å
Breadth: 3.886 Å
L/B Ratio: 1.382

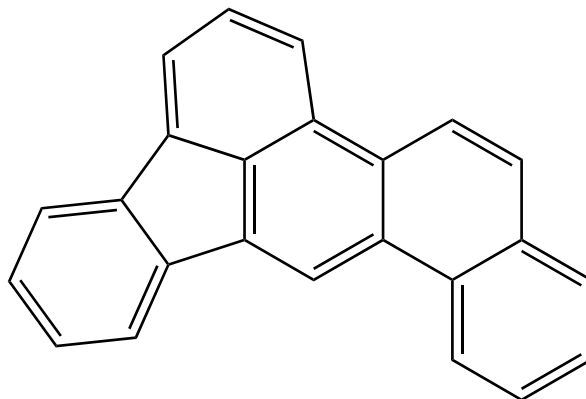
Cartesian coordinates:

C	3.6079	-2.9699	0.0000	C	0.8375	-0.3453	0.0000	H	5.3362	-0.0183	0.0000
C	4.6832	-2.0929	0.0000	C	-0.5182	-0.6336	0.0000	H	1.4364	-3.1893	0.0000
C	4.4852	-0.7067	0.0000	C	-1.4440	0.4637	0.0000	H	4.2990	2.5516	0.0000
C	2.2906	-2.4974	0.0000	C	-2.3359	-2.2484	0.0000	H	2.7837	4.5155	0.0000
C	2.0792	-1.1328	0.0000	C	-1.0125	-1.9872	0.0000	H	0.3219	4.2742	0.0000
C	3.1906	-0.2297	0.0000	C	-3.3016	-1.1774	0.0000	H	-1.7491	2.6021	0.0000
C	2.6717	1.1435	0.0000	C	-2.8690	0.1601	0.0000	H	-2.7095	-3.2789	0.0000
C	3.2161	2.3934	0.0000	C	-3.8347	1.1846	0.0000	H	-0.2675	-2.7985	0.0000
C	2.3336	3.5165	0.0000	C	-5.1818	0.8861	0.0000	H	-3.4953	2.2317	0.0000
C	0.9693	3.3908	0.0000	C	-5.6073	-0.4480	0.0000	H	-5.9233	1.6916	0.0000
C	1.2425	1.0130	0.0000	C	-4.6785	-1.4685	0.0000	H	-6.6781	-0.6759	0.0000
C	0.3661	2.0953	0.0000	H	3.7884	-4.0499	0.0000	H	-5.0059	-2.5145	0.0000
C	-1.0086	1.7869	0.0000	H	5.7048	-2.4872	0.0000				

Table 3.226: Table of thermodynamic data as a function of temperature for Dibenz[*a,j*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-45.323	433.602	433.602	∞
100	100.678	341.454	730.694	-38.924	456.738	495.386	-258.758
200	194.400	438.314	560.393	-24.416	444.564	538.872	-140.736
250	249.634	487.575	540.881	-13.327	438.777	563.118	-117.655
298.15	303.811	536.184	536.184	0.000	433.602	587.547	-102.934
300	305.871	538.070	536.190	0.564	433.411	588.501	-102.465
350	360.108	589.333	540.114	17.227	428.626	614.739	-91.743
400	410.473	640.756	549.482	36.510	424.462	641.609	-83.784
450	456.123	691.787	562.465	58.195	420.849	668.974	-77.651
500	496.939	741.998	577.916	82.041	417.709	696.733	-72.786
600	565.395	838.899	613.410	135.294	412.587	753.046	-65.557
700	619.547	930.281	652.218	194.644	408.819	810.110	-60.450
800	662.998	1015.948	692.389	258.848	406.247	867.617	-56.648
900	698.426	1096.152	732.844	326.977	404.719	925.377	-53.706
1000	727.710	1171.302	772.973	398.329	404.090	983.269	-51.360
1100	752.178	1241.841	812.424	472.359	404.191	1041.196	-49.441
1200	772.796	1308.198	851.002	548.636	404.899	1099.070	-47.840
1300	790.297	1370.765	888.600	626.814	406.054	1156.876	-46.483
1400	805.244	1429.893	925.172	706.611	407.542	1214.583	-45.316
1500	818.083	1485.898	960.703	787.793	409.293	1272.176	-44.300
1600	829.170	1539.059	995.203	870.169	411.192	1329.638	-43.407
1700	838.793	1589.622	1028.694	953.578	413.175	1386.958	-42.615
1800	847.184	1637.809	1061.206	1037.886	415.177	1444.217	-41.909
1900	854.536	1683.815	1092.773	1122.980	417.171	1501.318	-41.273
2000	861.006	1727.815	1123.433	1208.764	419.109	1558.338	-40.699
2100	866.723	1769.965	1153.224	1295.156	420.923	1615.252	-40.176
2200	871.794	1810.405	1182.183	1382.087	422.613	1672.084	-39.700
2300	876.311	1849.259	1210.347	1469.497	424.174	1728.842	-39.262
2400	880.348	1886.641	1237.752	1557.334	425.543	1785.493	-38.859
2500	883.969	1922.654	1264.432	1645.553	426.732	1842.191	-38.490
2600	887.228	1957.388	1290.421	1734.115	427.709	1898.742	-38.145
2700	890.169	1990.928	1315.748	1822.988	428.477	1955.324	-37.827
2800	892.833	2023.351	1340.444	1912.140	429.015	2011.900	-37.532
2900	895.251	2054.724	1364.536	2001.546	429.295	2068.415	-37.255
3000	897.452	2085.112	1388.051	2091.183	429.357	2124.947	-36.998
3100	899.462	2114.573	1411.015	2181.030	429.132	2181.414	-36.756
3200	901.301	2143.159	1433.450	2271.070	428.657	2237.956	-36.530
3300	902.987	2170.920	1455.379	2361.285	427.917	2294.553	-36.319
3400	904.537	2197.900	1476.823	2451.662	426.886	2351.099	-36.120
3500	905.965	2224.141	1497.802	2542.189	425.569	2407.664	-35.932
3600	907.284	2249.682	1518.334	2632.852	423.986	2464.348	-35.756
3700	908.503	2274.557	1538.438	2723.642	422.108	2521.095	-35.591
3800	909.632	2298.801	1558.130	2814.549	419.912	2577.843	-35.434
3900	910.681	2322.442	1577.426	2905.566	417.435	2634.607	-35.286
4000	911.656	2345.511	1596.340	2996.683	414.663	2691.562	-35.147
4100	912.564	2368.034	1614.889	3087.895	411.563	2748.524	-35.016
4200	913.410	2390.035	1633.084	3179.194	408.162	2805.557	-34.891
4300	914.202	2411.537	1650.938	3270.575	404.445	2862.596	-34.773
4400	914.942	2432.563	1668.464	3362.032	400.421	2919.806	-34.662
4500	915.635	2453.132	1685.674	3453.562	396.103	2977.161	-34.557
4600	916.285	2473.264	1702.577	3545.158	391.446	3034.621	-34.458
4700	916.896	2492.976	1719.185	3636.817	386.461	3092.086	-34.364
4800	917.471	2512.286	1735.508	3728.536	381.191	3149.754	-34.276
4900	918.012	2531.209	1751.554	3820.310	375.569	3207.416	-34.191
5000	918.522	2549.761	1767.333	3912.137	369.679	3265.361	-34.112

3.227. Indeno[1,2,3-*hi*]chrysene



Other names: Naphtho[1,2-*b*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 111189-32-3

Point Group: C_s

Length: 14.93 Å

Width: 10.66 Å

Breadth: 3.885 Å

L/B Ratio: 1.401

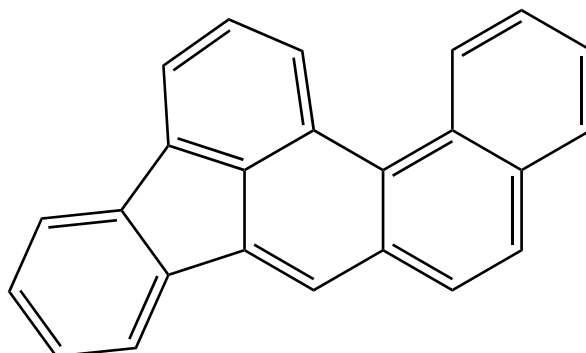
Cartesian coordinates:

C	5.1462	1.5580	0.0000	C	0.1309	-1.7470	0.0000	H	2.1748	3.2522	0.0000
C	4.2566	2.6225	0.0000	C	0.4710	-3.1238	0.0000	H	5.3956	-0.6031	0.0000
C	2.8724	2.4089	0.0000	C	1.7936	-3.5103	0.0000	H	-0.3819	2.1919	0.0000
C	4.6901	0.2337	0.0000	C	2.8636	-2.5787	0.0000	H	-4.4666	-2.1683	0.0000
C	3.3287	0.0102	0.0000	C	2.5597	-1.2418	0.0000	H	-2.1472	-3.1136	0.0000
C	2.4105	1.1089	0.0000	C	-3.7886	-0.0976	0.0000	H	-0.3476	-3.8574	0.0000
C	1.0420	0.5746	0.0000	C	-2.6789	0.7694	0.0000	H	2.0401	-4.5777	0.0000
C	-0.2082	1.1055	0.0000	C	-2.9095	2.1673	0.0000	H	3.8998	-2.9307	0.0000
C	-1.1896	-1.1729	0.0000	C	-4.1864	2.6697	0.0000	H	-2.0402	2.8422	0.0000
C	-1.3453	0.2214	0.0000	C	-5.2930	1.7981	0.0000	H	-4.3556	3.7514	0.0000
C	-3.5881	-1.5130	0.0000	C	-5.0990	0.4395	0.0000	H	-6.3052	2.2153	0.0000
C	-2.3311	-2.0286	0.0000	H	6.2239	1.7519	0.0000	H	-5.9540	-0.2462	0.0000
C	1.1888	-0.8551	0.0000	H	4.6389	3.6487	0.0000				

Table 3.227: Table of thermodynamic data as a function of temperature for Indeno[1,2,3-*hi*]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-45.168	412.626	412.626	∞
100	100.605	338.786	727.165	-38.838	435.848	474.764	-247.986
200	193.904	435.478	557.261	-24.357	423.648	518.523	-135.421
250	249.018	484.613	537.796	-13.296	417.833	542.913	-113.433
298.15	303.157	533.109	533.109	0.000	412.626	567.489	-99.420
300	305.217	534.991	533.115	0.563	412.434	568.448	-98.974
350	359.463	586.154	537.032	17.193	407.617	594.842	-88.774
400	409.859	637.493	546.382	36.444	403.422	621.874	-81.207
450	455.552	688.453	559.342	58.100	399.778	649.404	-75.379
500	496.414	738.607	574.769	81.919	396.611	677.331	-70.759
600	564.964	835.421	610.215	135.124	391.441	733.987	-63.898
700	619.201	926.742	648.978	194.435	387.634	791.403	-59.054
800	662.723	1012.368	689.109	258.608	385.032	849.265	-55.450
900	698.209	1092.543	729.529	326.712	383.479	907.385	-52.662
1000	727.540	1167.672	769.627	398.045	382.831	965.639	-50.439
1100	752.044	1238.197	809.052	472.060	382.917	1023.930	-48.621
1200	772.691	1304.544	847.606	548.325	383.613	1082.169	-47.105
1300	790.213	1367.103	885.185	626.494	384.758	1140.340	-45.818
1400	805.177	1426.226	921.738	706.283	386.239	1198.414	-44.712
1500	818.030	1482.227	957.254	787.459	387.984	1256.374	-43.750
1600	829.127	1535.384	991.740	869.830	389.878	1314.204	-42.903
1700	838.758	1585.945	1025.218	953.236	391.857	1371.891	-42.152
1800	847.156	1634.131	1057.719	1037.541	393.856	1429.518	-41.483
1900	854.514	1680.135	1089.276	1122.632	395.848	1486.987	-40.879
2000	860.987	1724.134	1119.927	1208.414	397.784	1544.375	-40.334
2100	866.707	1766.283	1149.710	1294.805	399.596	1601.657	-39.838
2200	871.782	1806.722	1178.661	1381.734	401.285	1658.857	-39.385
2300	876.301	1845.576	1206.818	1469.143	402.844	1715.983	-38.970
2400	880.340	1882.958	1234.217	1556.978	404.213	1773.003	-38.588
2500	883.962	1918.970	1260.891	1645.197	405.401	1830.069	-38.236
2600	887.222	1953.704	1286.874	1733.759	406.377	1886.989	-37.909
2700	890.164	1987.244	1312.196	1822.630	407.145	1943.939	-37.607
2800	892.828	2019.666	1336.887	1911.782	407.682	2000.884	-37.326
2900	895.247	2051.040	1360.975	2001.188	407.961	2057.767	-37.064
3000	897.449	2081.428	1384.486	2090.825	408.023	2114.667	-36.819
3100	899.459	2110.888	1407.446	2180.671	407.798	2171.502	-36.589
3200	901.299	2139.474	1429.877	2270.711	407.323	2228.414	-36.374
3300	902.986	2167.235	1451.803	2360.926	406.583	2285.379	-36.174
3400	904.536	2194.215	1473.243	2451.303	405.552	2342.294	-35.984
3500	905.964	2220.456	1494.219	2541.829	404.235	2399.227	-35.806
3600	907.283	2245.997	1514.749	2632.493	402.651	2456.279	-35.639
3700	908.502	2270.872	1534.850	2723.283	400.773	2513.395	-35.482
3800	909.632	2295.115	1554.539	2814.190	398.577	2570.511	-35.333
3900	910.680	2318.757	1573.833	2905.206	396.101	2627.644	-35.193
4000	911.655	2341.826	1592.745	2996.324	393.328	2684.967	-35.061
4100	912.563	2364.349	1611.291	3087.535	390.228	2742.297	-34.937
4200	913.410	2386.349	1629.484	3178.834	386.827	2799.699	-34.819
4300	914.202	2407.852	1647.337	3270.215	383.110	2857.107	-34.706
4400	914.942	2428.877	1664.861	3361.673	379.086	2914.685	-34.601
4500	915.635	2449.447	1682.068	3453.202	374.768	2972.408	-34.502
4600	916.286	2469.579	1698.970	3544.798	370.111	3030.238	-34.409
4700	916.897	2489.291	1715.577	3636.458	365.126	3088.071	-34.319
4800	917.471	2508.601	1731.897	3728.176	359.856	3146.108	-34.236
4900	918.012	2527.524	1747.942	3819.951	354.234	3204.138	-34.156
5000	918.522	2546.076	1763.720	3911.778	348.344	3262.451	-34.082

3.228. Naphtho[2,1-*b*]fluoranthene



Other names: Dibenz[*e,l*]acephenanthrylene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 40563-35-7

Point Group: C₁

Length: 15.48 Å

Width: 9.880 Å

Breadth: 4.613 Å

L/B Ratio: 1.567

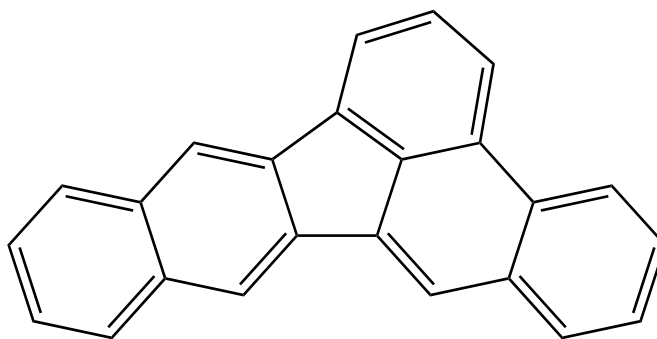
Cartesian coordinates:

C	3.3023	-1.3209	0.4374	C	0.3229	-0.8805	-0.1126	H	-3.5185	2.9231	0.2233
C	2.7454	-0.0696	0.0725	C	-2.1278	-1.3523	-0.0714	H	-4.9877	-1.8772	0.0239
C	3.6447	1.0017	-0.1173	C	-3.3231	-0.5058	0.0298	H	-0.7816	2.9372	-0.0390
C	5.0431	0.7839	-0.0737	C	-2.9054	0.8596	0.0876	H	1.5028	-2.6888	-0.4582
C	5.5455	-0.4587	0.2176	C	-3.8342	1.8760	0.1804	H	-0.4014	-4.2098	-0.4972
C	4.6601	-1.5135	0.5035	C	-5.1912	1.5324	0.2188	H	-2.7459	-3.4120	-0.2397
C	3.1526	2.3289	-0.3060	C	-5.5970	0.2065	0.1641	H	1.4365	3.5959	-0.3320
C	1.8200	2.5720	-0.2468	C	-4.6634	-0.8327	0.0679	H	3.8706	3.1415	-0.4652
C	0.8815	1.5020	-0.1017	C	-1.9171	-2.6982	-0.2124	H	5.7177	1.6257	-0.2683
C	1.3236	0.1670	-0.0460	C	-0.5796	-3.1392	-0.3469	H	6.6257	-0.6331	0.2480
C	-0.5065	1.8762	-0.0375	C	0.4954	-2.2782	-0.3098	H	5.0644	-2.4905	0.7885
C	-1.4398	0.8961	0.0269	H	-6.6645	-0.0354	0.1963	H	2.6402	-2.1554	0.7031
C	-1.0047	-0.4728	-0.0391	H	-5.9416	2.3264	0.2936				

Table 3.228: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*b*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.774	433.125	433.125	∞
100	98.740	334.373	720.489	-38.612	456.574	495.930	-259.042
200	192.834	430.021	551.402	-24.276	444.227	540.193	-141.081
250	248.212	478.948	531.994	-13.262	438.366	564.863	-118.019
298.15	302.537	527.319	527.319	0.000	433.125	589.714	-103.313
300	304.604	529.197	527.325	0.562	432.932	590.684	-102.845
350	358.998	580.277	531.235	17.165	428.088	617.370	-92.136
400	409.511	631.562	540.571	36.396	423.873	644.698	-84.187
450	455.293	682.486	553.516	58.037	420.214	672.524	-78.063
500	496.222	732.616	568.928	81.844	417.036	700.751	-73.205
600	564.856	829.404	604.346	135.035	411.851	758.008	-65.989
700	619.135	920.712	643.087	194.337	408.036	816.025	-60.891
800	662.675	1006.331	683.200	258.505	405.428	874.492	-57.097
900	698.169	1086.500	723.606	326.605	403.871	933.215	-54.161
1000	727.502	1161.625	763.692	397.934	403.219	992.074	-51.820
1100	752.007	1232.147	803.106	471.945	403.302	1050.969	-49.905
1200	772.654	1298.491	841.651	548.207	403.993	1109.813	-48.308
1300	790.176	1361.047	879.222	626.372	405.135	1168.591	-46.954
1400	805.141	1420.167	915.769	706.157	406.612	1227.270	-45.789
1500	817.994	1476.165	951.279	787.330	408.353	1285.836	-44.776
1600	829.093	1529.320	985.759	869.697	410.244	1344.272	-43.885
1700	838.725	1579.879	1019.233	953.100	412.220	1402.566	-43.095
1800	847.124	1628.063	1051.729	1037.401	414.216	1460.799	-42.390
1900	854.483	1674.066	1083.282	1122.490	416.204	1518.875	-41.756
2000	860.958	1718.063	1113.929	1208.269	418.137	1576.870	-41.183
2100	866.679	1760.211	1143.708	1294.656	419.947	1634.759	-40.662
2200	871.755	1800.648	1172.656	1381.583	421.632	1692.567	-40.186
2300	876.276	1839.501	1200.810	1468.989	423.189	1750.301	-39.750
2400	880.316	1876.882	1228.206	1556.822	424.555	1807.928	-39.348
2500	883.940	1912.893	1254.878	1645.038	425.741	1865.602	-38.979
2600	887.200	1947.626	1280.858	1733.598	426.715	1923.129	-38.635
2700	890.144	1981.166	1306.178	1822.468	427.481	1980.687	-38.318
2800	892.809	2013.587	1330.866	1911.617	428.016	2038.240	-38.023
2900	895.229	2044.960	1354.952	2001.021	428.294	2095.731	-37.747
3000	897.432	2075.347	1378.462	2090.656	428.353	2153.239	-37.490
3100	899.443	2104.807	1401.420	2180.501	428.127	2210.682	-37.249
3200	901.283	2133.393	1423.849	2270.539	427.650	2268.202	-37.024
3300	902.970	2161.153	1445.773	2360.753	426.908	2325.775	-36.813
3400	904.522	2188.132	1467.212	2451.128	425.876	2383.298	-36.614
3500	905.951	2214.373	1488.187	2541.653	424.557	2440.840	-36.427
3600	907.270	2239.913	1508.715	2632.315	422.972	2498.500	-36.252
3700	908.490	2264.789	1528.815	2723.104	421.093	2556.224	-36.087
3800	909.620	2289.032	1548.503	2814.010	418.896	2613.949	-35.930
3900	910.669	2312.673	1567.795	2905.025	416.418	2671.691	-35.783
4000	911.644	2335.742	1586.706	2996.141	413.645	2729.622	-35.644
4100	912.553	2358.264	1605.251	3087.352	410.544	2787.561	-35.513
4200	913.400	2380.264	1623.443	3178.650	407.141	2845.571	-35.389
4300	914.192	2401.767	1641.295	3270.030	403.423	2903.587	-35.271
4400	914.932	2422.792	1658.818	3361.486	399.399	2961.774	-35.160
4500	915.626	2443.361	1676.024	3453.015	395.080	3020.106	-35.056
4600	916.277	2463.493	1692.925	3544.610	390.422	3078.544	-34.957
4700	916.888	2483.205	1709.531	3636.269	385.436	3136.986	-34.863
4800	917.463	2502.515	1725.851	3727.987	380.165	3195.631	-34.775
4900	918.004	2521.438	1741.895	3819.760	374.543	3254.269	-34.690
5000	918.515	2539.989	1757.672	3911.586	368.652	3313.192	-34.612

3.229. Naphth[2,3-*e*]acephenanthrylene



Other names: Dibenzo[*b,k*]fluoranthene
Dibenzo-2,3,11,12-fluoranthene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol

CAS Number: 205-97-0

Point Group: C_s

Length: 16.10 Å

Width: 10.22 Å

Breadth: 3.884 Å

L/B Ratio: 1.575

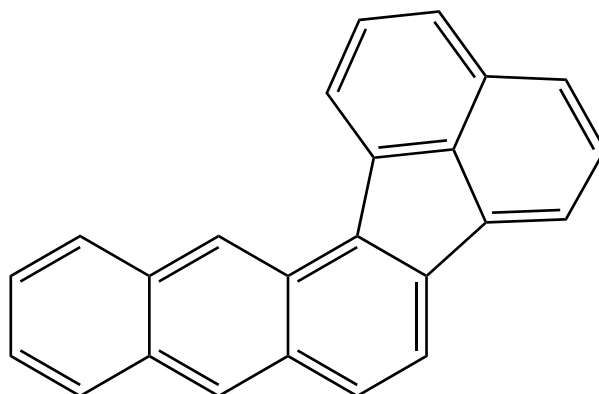
Cartesian coordinates:

C	5.9807	0.3746	0.0000	C	-2.8253	1.2787	0.0000	H	4.0066	3.1594	0.0000
C	5.6168	1.7379	0.0000	C	-3.7788	2.3193	0.0000	H	5.2932	-1.6603	0.0000
C	4.2950	2.1021	0.0000	C	-5.1271	2.0370	0.0000	H	1.6272	2.5539	0.0000
C	5.0163	-0.5999	0.0000	C	-5.5731	0.7062	0.0000	H	2.9279	-2.3213	0.0000
C	3.6421	-0.2501	0.0000	C	-4.6627	-0.3272	0.0000	H	-1.1136	2.6601	0.0000
C	3.2780	1.1141	0.0000	C	-0.9812	-0.7667	0.0000	H	-3.4335	3.3597	0.0000
C	1.8994	1.4926	0.0000	C	-2.3149	-1.1372	0.0000	H	-5.8602	2.8503	0.0000
C	2.6356	-1.2654	0.0000	C	-2.5827	-2.5260	0.0000	H	-6.6476	0.4962	0.0000
C	1.3279	-0.8894	0.0000	C	-1.5420	-3.4337	0.0000	H	-4.9904	-1.3763	0.0000
C	0.9528	0.5150	0.0000	C	-0.1848	-3.0355	0.0000	H	-3.6299	-2.8570	0.0000
C	-0.5129	0.5986	0.0000	C	0.0978	-1.6909	0.0000	H	-1.7672	-4.5058	0.0000
C	-1.4166	1.6073	0.0000	H	7.0420	0.1054	0.0000	H	0.6117	-3.7861	0.0000
C	-3.2800	-0.0604	0.0000	H	6.4027	2.5002	0.0000				

Table 3.229: Table of thermodynamic data as a function of temperature for Naphth[2,3-*e*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.905	404.006	404.006	∞
100	99.126	335.906	722.930	-38.702	427.364	466.567	-243.704
200	193.296	431.855	553.471	-24.323	415.061	510.660	-133.368
250	248.698	480.888	534.028	-13.285	409.223	535.235	-111.829
298.15	303.013	529.344	529.344	0.000	404.006	559.991	-98.106
300	305.078	531.225	529.350	0.562	403.814	560.958	-97.669
350	359.419	582.375	533.266	17.188	398.992	587.540	-87.684
400	409.857	633.711	542.614	36.439	394.796	614.761	-80.278
450	455.566	684.672	555.573	58.095	391.153	642.480	-74.576
500	496.434	734.827	570.999	81.914	387.987	670.596	-70.055
600	564.992	831.646	606.443	135.122	382.819	727.630	-63.345
700	619.248	922.973	645.206	194.437	379.016	785.423	-58.608
800	662.794	1008.607	685.338	258.615	376.420	843.662	-55.084
900	698.304	1088.791	725.760	326.728	374.875	902.157	-52.359
1000	727.654	1163.932	765.860	398.071	374.238	960.786	-50.185
1100	752.171	1234.469	805.288	472.098	374.336	1019.450	-48.409
1200	772.827	1300.827	843.846	548.377	375.044	1078.061	-46.926
1300	790.353	1363.397	881.428	626.560	376.204	1136.604	-45.668
1400	805.318	1422.530	917.985	706.363	377.699	1195.048	-44.587
1500	818.169	1478.541	953.505	787.553	379.457	1253.377	-43.646
1600	829.263	1531.707	987.996	869.938	381.365	1311.575	-42.818
1700	838.889	1582.276	1021.478	953.357	383.358	1369.630	-42.083
1800	847.282	1630.469	1053.983	1037.675	385.370	1427.623	-41.428
1900	854.634	1676.480	1085.544	1122.778	387.374	1485.457	-40.837
2000	861.102	1720.485	1116.199	1208.572	389.321	1543.211	-40.304
2100	866.816	1762.639	1145.985	1294.974	391.145	1600.857	-39.818
2200	871.885	1803.083	1174.940	1381.914	392.844	1658.422	-39.375
2300	876.399	1841.941	1203.101	1469.332	394.413	1715.912	-38.969
2400	880.432	1879.327	1230.503	1557.177	395.792	1773.295	-38.594
2500	884.050	1915.343	1257.181	1645.405	396.989	1830.724	-38.250
2600	887.305	1950.081	1283.167	1733.975	397.974	1888.006	-37.930
2700	890.243	1983.624	1308.492	1822.855	398.749	1945.318	-37.634
2800	892.903	2016.049	1333.186	1912.015	399.294	2002.625	-37.359
2900	895.318	2047.425	1357.277	2001.428	399.581	2059.870	-37.101
3000	897.517	2077.815	1380.791	2091.071	399.649	2117.131	-36.862
3100	899.524	2107.278	1403.754	2180.925	399.431	2174.328	-36.636
3200	901.360	2135.866	1426.188	2270.970	398.962	2231.600	-36.426
3300	903.044	2163.628	1448.116	2361.192	398.228	2288.926	-36.230
3400	904.591	2190.610	1469.559	2451.574	397.203	2346.201	-36.044
3500	906.017	2216.853	1490.537	2542.106	395.891	2403.495	-35.869
3600	907.333	2242.395	1511.069	2632.774	394.312	2460.908	-35.706
3700	908.550	2267.272	1531.172	2723.569	392.439	2518.383	-35.552
3800	909.678	2291.516	1550.863	2814.481	390.248	2575.860	-35.407
3900	910.724	2315.159	1570.159	2905.502	387.776	2633.352	-35.269
4000	911.697	2338.229	1589.073	2996.624	385.008	2691.035	-35.141
4100	912.604	2360.753	1607.621	3087.839	381.912	2748.725	-35.018
4200	913.449	2382.754	1625.816	3179.142	378.515	2806.487	-34.903
4300	914.239	2404.258	1643.670	3270.527	374.801	2864.253	-34.793
4400	914.977	2425.284	1661.196	3361.988	370.782	2922.191	-34.690
4500	915.669	2445.854	1678.405	3453.521	366.467	2980.274	-34.593
4600	916.318	2465.987	1695.308	3545.121	361.813	3038.462	-34.502
4700	916.928	2485.700	1711.916	3636.783	356.832	3096.655	-34.415
4800	917.501	2505.010	1728.238	3728.505	351.564	3155.051	-34.333
4900	918.041	2523.934	1744.285	3820.283	345.946	3213.440	-34.255
5000	918.550	2542.486	1760.064	3912.112	340.059	3272.112	-34.183

3.230. Naphtho[2,3-*j*]fluoranthene



Other names: Acenaphth[1,2-*a*]anthracene
Naphtho(2',3':7,8)fluoranthene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 205-83-4
Point Group: C_s

Length: 15.35 Å
Width: 9.843 Å
Breadth: 3.888 Å
L/B Ratio: 1.560

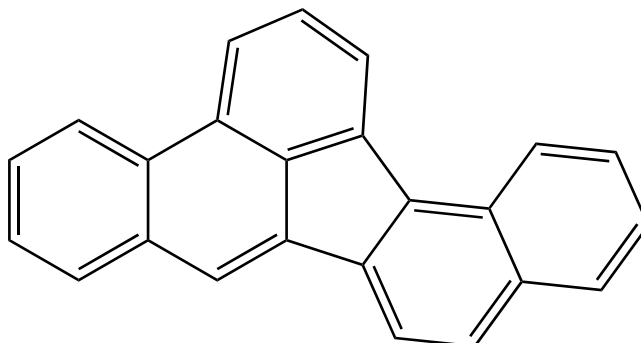
Cartesian coordinates:

C	-0.5276	0.2752	0.0000	C	-0.7105	2.7201	0.0000	H	5.5667	1.7393	0.0000
C	-1.3052	1.4392	0.0000	C	-1.4206	-0.8933	0.0000	H	3.4865	-2.8079	0.0000
C	5.3035	-1.6739	0.0000	C	-3.7114	-2.5390	0.0000	H	3.3367	2.7612	0.0000
C	5.8966	-0.3768	0.0000	C	-2.4400	-3.0632	0.0000	H	1.2421	-1.7870	0.0000
C	5.1199	0.7386	0.0000	C	-1.2708	-2.2533	0.0000	H	1.1406	3.7945	0.0000
C	3.9518	-1.8158	0.0000	C	-3.9016	-1.1285	0.0000	H	-1.3487	3.6096	0.0000
C	3.0982	-0.6632	0.0000	C	-2.7466	-0.3593	0.0000	H	-4.5888	-3.1944	0.0000
C	3.6897	0.6310	0.0000	C	-2.7279	1.0699	0.0000	H	-2.3071	-4.1508	0.0000
C	2.8776	1.7647	0.0000	C	-3.9221	1.7357	0.0000	H	-0.2703	-2.7094	0.0000
C	1.7100	-0.7886	0.0000	C	-5.1208	0.9675	0.0000	H	-3.9723	2.8290	0.0000
C	0.8929	0.3473	0.0000	C	-5.1291	-0.4072	0.0000	H	-6.0731	1.5096	0.0000
C	1.4825	1.6462	0.0000	H	5.9597	-2.5503	0.0000	H	-6.0726	-0.9632	0.0000
C	0.6522	2.8131	0.0000	H	6.9888	-0.3000	0.0000				

Table 3.230: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*j*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.969	443.073	443.073	∞
100	98.853	339.026	725.913	-38.689	466.444	505.335	-263.955
200	193.284	434.802	556.465	-24.333	454.118	549.128	-143.415
250	248.817	483.848	537.012	-13.291	448.284	573.556	-119.835
298.15	303.134	532.327	532.327	0.000	443.073	598.168	-104.794
300	305.197	534.209	532.333	0.563	442.881	599.129	-104.316
350	359.489	585.373	536.250	17.193	438.064	625.563	-93.358
400	409.874	636.715	545.600	36.446	433.870	652.633	-85.223
450	455.542	687.676	558.561	58.102	430.227	680.202	-78.954
500	496.381	737.827	573.988	81.919	427.058	708.168	-73.980
600	564.911	834.633	609.433	135.120	421.884	764.902	-66.589
700	619.154	925.946	648.195	194.426	418.072	822.397	-61.367
800	662.693	1011.568	688.324	258.595	415.466	880.340	-57.479
900	698.199	1091.740	728.743	326.698	413.911	938.539	-54.470
1000	727.547	1166.869	768.839	398.030	413.263	996.874	-52.070
1100	752.065	1237.396	808.263	472.046	413.350	1055.245	-50.108
1200	772.723	1303.745	846.816	548.315	414.049	1113.564	-48.471
1300	790.252	1366.306	884.394	626.487	415.198	1171.815	-47.083
1400	805.221	1425.433	920.947	706.280	416.683	1229.969	-45.890
1500	818.076	1481.436	956.463	787.461	418.432	1288.008	-44.851
1600	829.174	1534.597	990.949	869.836	420.330	1345.916	-43.939
1700	838.805	1585.161	1024.428	953.247	422.315	1403.682	-43.129
1800	847.203	1633.349	1056.929	1037.556	424.318	1461.387	-42.407
1900	854.559	1679.356	1088.486	1122.653	426.315	1518.934	-41.758
2000	861.031	1723.357	1119.138	1208.439	428.255	1576.400	-41.171
2100	866.750	1765.508	1148.921	1294.834	430.072	1633.759	-40.637
2200	871.823	1805.949	1177.873	1381.767	431.764	1691.038	-40.150
2300	876.340	1844.805	1206.031	1469.180	433.328	1748.241	-39.703
2400	880.377	1882.188	1233.430	1557.019	434.700	1805.338	-39.291
2500	883.998	1918.202	1260.105	1645.241	435.892	1862.481	-38.914
2600	887.256	1952.937	1286.088	1733.807	436.872	1919.477	-38.562
2700	890.197	1986.479	1311.411	1822.682	437.643	1976.503	-38.237
2800	892.860	2018.902	1336.103	1911.837	438.183	2033.525	-37.935
2900	895.277	2050.276	1360.192	2001.246	438.466	2090.484	-37.653
3000	897.478	2080.665	1383.704	2090.885	438.530	2147.461	-37.390
3100	899.486	2110.127	1406.664	2180.735	438.308	2204.372	-37.143
3200	901.324	2138.714	1429.096	2270.777	437.836	2261.360	-36.912
3300	903.010	2166.475	1451.022	2360.995	437.098	2318.401	-36.696
3400	904.560	2193.456	1472.464	2451.374	436.069	2375.392	-36.493
3500	905.987	2219.698	1493.440	2541.903	434.755	2432.401	-36.301
3600	907.304	2245.239	1513.970	2632.568	433.173	2489.529	-36.121
3700	908.523	2270.115	1534.072	2723.360	431.297	2546.720	-35.953
3800	909.651	2294.359	1553.762	2814.270	429.103	2603.912	-35.793
3900	910.699	2318.001	1573.056	2905.288	426.629	2661.121	-35.641
4000	911.673	2341.071	1591.969	2996.407	423.858	2718.520	-35.499
4100	912.581	2363.593	1610.515	3087.620	420.760	2775.925	-35.365
4200	913.427	2385.595	1628.709	3178.921	417.360	2833.403	-35.238
4300	914.217	2407.097	1646.562	3270.304	413.645	2890.886	-35.117
4400	914.957	2428.123	1664.086	3361.763	409.623	2948.540	-35.003
4500	915.650	2448.693	1681.294	3453.294	405.306	3006.338	-34.896
4600	916.300	2468.825	1698.197	3544.891	400.650	3064.243	-34.795
4700	916.910	2488.538	1714.803	3636.552	395.667	3122.152	-34.698
4800	917.484	2507.848	1731.125	3728.272	390.398	3180.263	-34.608
4900	918.025	2526.772	1747.170	3820.048	384.778	3238.369	-34.521
5000	918.534	2545.323	1762.948	3911.876	378.889	3296.758	-34.440

3.231. Naphth[1,2-*e*]acephenanthrylene



Other names: Dibenzo[*b,j*]fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 5385-22-8

Point Group: C_s

Length: 15.78 Å

Width: 9.910 Å

Breadth: 3.888 Å

L/B Ratio: 1.592

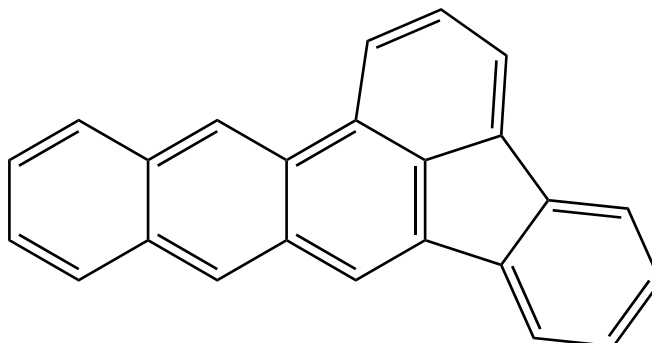
Cartesian coordinates:

C	5.5811	-0.0260	0.0000	C	-0.4792	-1.1257	0.0000	H	4.0657	3.0267	0.0000
C	5.4336	1.3694	0.0000	C	-1.4914	-0.0586	0.0000	H	4.5655	-1.9331	0.0000
C	4.1779	1.9362	0.0000	C	-0.8350	1.1876	0.0000	H	1.6519	2.8482	0.0000
C	4.4687	-0.8386	0.0000	C	-1.5556	2.3897	0.0000	H	-1.4513	-3.0484	0.0000
C	3.1762	-0.2801	0.0000	C	-2.9301	2.3363	0.0000	H	0.7171	-4.2849	0.0000
C	3.0222	1.1263	0.0000	C	-2.9004	-0.1256	0.0000	H	2.8980	-3.0945	0.0000
C	1.7186	1.7546	0.0000	C	-3.6183	1.0958	0.0000	H	-1.0212	3.3453	0.0000
C	2.0001	-1.1223	0.0000	C	-5.0420	1.0560	0.0000	H	-3.5167	3.2623	0.0000
C	-0.4983	-2.5005	0.0000	C	-5.7034	-0.1399	0.0000	H	-5.5954	2.0021	0.0000
C	0.7357	-3.1895	0.0000	C	-4.9827	-1.3596	0.0000	H	-6.7978	-0.1710	0.0000
C	1.9530	-2.5357	0.0000	C	-3.6165	-1.3554	0.0000	H	-5.5369	-2.3038	0.0000
C	0.7811	-0.4681	0.0000	H	6.5847	-0.4636	0.0000	H	-3.0413	-2.2944	0.0000
C	0.6177	0.9664	0.0000	H	6.3250	2.0053	0.0000				

Table 3.231: Table of thermodynamic data as a function of temperature for Naphth[1,2-*e*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.033	416.251	416.251	∞
100	99.787	337.200	724.776	-38.758	439.553	478.627	-250.004
200	193.564	433.475	555.143	-24.334	427.295	522.571	-136.479
250	248.794	482.548	535.693	-13.286	421.466	547.063	-114.300
298.15	302.982	531.010	531.010	0.000	416.251	571.739	-100.164
300	305.044	532.891	531.016	0.562	416.058	572.702	-99.714
350	359.312	584.029	534.931	17.184	411.233	599.202	-89.424
400	409.723	635.349	544.277	36.429	407.030	626.341	-81.790
450	455.429	686.294	557.232	58.078	403.381	653.978	-75.910
500	496.304	736.435	572.653	81.891	400.208	682.014	-71.248
600	564.876	833.231	608.088	135.086	395.028	738.888	-64.325
700	619.131	924.540	646.841	194.389	391.213	796.523	-59.436
800	662.666	1010.158	686.963	258.556	388.605	854.606	-55.799
900	698.162	1090.327	727.376	326.655	387.046	912.947	-52.985
1000	727.500	1165.451	767.468	397.984	386.394	971.423	-50.741
1100	752.009	1235.973	806.887	471.995	386.477	1029.936	-48.907
1200	772.660	1302.317	845.436	548.257	387.169	1088.397	-47.376
1300	790.186	1364.874	883.010	626.423	388.312	1146.792	-46.078
1400	805.153	1423.995	919.560	706.209	389.790	1205.089	-44.961
1500	818.008	1479.994	955.072	787.383	391.532	1263.272	-43.990
1600	829.107	1533.150	989.555	869.752	393.424	1321.325	-43.136
1700	838.740	1583.710	1023.030	953.156	395.401	1379.236	-42.378
1800	847.140	1631.894	1055.528	1037.459	397.399	1437.086	-41.702
1900	854.498	1677.898	1087.083	1122.549	399.389	1494.779	-41.093
2000	860.973	1721.896	1117.732	1208.329	401.323	1552.391	-40.543
2100	866.694	1764.044	1147.512	1294.719	403.134	1609.896	-40.043
2200	871.770	1804.483	1176.461	1381.647	404.821	1667.321	-39.586
2300	876.289	1843.336	1204.617	1469.054	406.380	1724.671	-39.168
2400	880.329	1880.717	1232.014	1556.889	407.747	1781.914	-38.782
2500	883.953	1916.729	1258.687	1645.106	408.935	1839.205	-38.427
2600	887.213	1951.463	1284.668	1733.667	409.910	1896.348	-38.097
2700	890.156	1985.003	1309.989	1822.538	410.677	1953.522	-37.792
2800	892.821	2017.424	1334.678	1911.689	411.213	2010.692	-37.509
2900	895.240	2048.798	1358.765	2001.094	411.492	2067.799	-37.244
3000	897.442	2079.185	1382.275	2090.730	411.552	2124.924	-36.997
3100	899.453	2108.646	1405.234	2180.576	411.327	2181.983	-36.765
3200	901.292	2137.231	1427.664	2270.615	410.851	2239.119	-36.549
3300	902.980	2164.992	1449.589	2360.829	410.110	2296.308	-36.347
3400	904.530	2191.972	1471.029	2451.206	409.079	2353.447	-36.156
3500	905.959	2218.213	1492.004	2541.731	407.761	2410.605	-35.976
3600	907.278	2243.753	1512.533	2632.394	406.177	2467.881	-35.807
3700	908.497	2268.629	1532.633	2723.184	404.298	2525.221	-35.649
3800	909.627	2292.872	1552.322	2814.091	402.102	2582.562	-35.499
3900	910.676	2316.514	1571.615	2905.106	399.625	2639.919	-35.357
4000	911.651	2339.582	1590.527	2996.223	396.852	2697.467	-35.225
4100	912.559	2362.105	1609.072	3087.434	393.752	2755.021	-35.099
4200	913.407	2384.105	1627.264	3178.733	390.350	2812.648	-34.980
4300	914.198	2405.608	1645.116	3270.114	386.633	2870.279	-34.866
4400	914.938	2426.633	1662.640	3361.571	382.609	2928.082	-34.760
4500	915.632	2447.202	1679.847	3453.100	378.291	2986.030	-34.660
4600	916.282	2467.334	1696.748	3544.696	373.633	3044.084	-34.566
4700	916.893	2487.047	1713.354	3636.355	368.648	3102.142	-34.476
4800	917.468	2506.356	1729.674	3728.073	363.377	3160.403	-34.391
4900	918.009	2525.280	1745.719	3819.848	357.755	3218.657	-34.311
5000	918.519	2543.831	1761.496	3911.674	351.865	3277.195	-34.236

3.232. Dibenz[*e,k*]acephenanthrylene



Other names: Naphtho[2',3':2,3]fluoranthene
Naphtho[2,3-*b*]fluoranthene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 206-06-4
Point Group: C_s

Length: 16.12 Å
Width: 10.02 Å
Breadth: 3.888 Å
L/B Ratio: 1.609

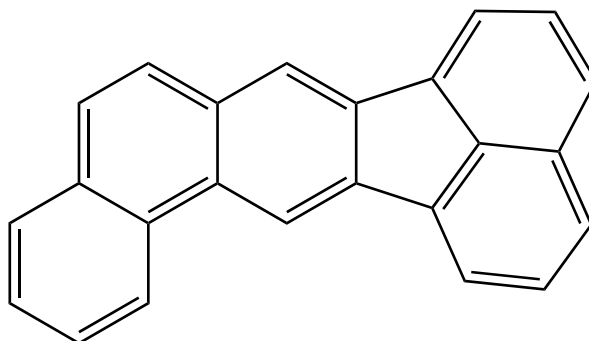
Cartesian coordinates:

C	5.9658	-0.0836	0.0000	C	-1.3558	-3.3925	0.0000	H	4.4966	3.0046	0.0000
C	5.8375	1.3304	0.0000	C	-0.1279	-2.7530	0.0000	H	4.9464	-1.9715	0.0000
C	4.6044	1.9140	0.0000	C	-1.2702	-0.6711	0.0000	H	2.0559	2.7854	0.0000
C	4.8574	-0.8793	0.0000	C	-1.4112	0.7720	0.0000	H	2.4844	-2.1952	0.0000
C	3.5540	-0.2991	0.0000	C	-2.5346	-1.3121	0.0000	H	-0.3575	2.6386	0.0000
C	3.4255	1.1095	0.0000	C	-3.5382	-0.2394	0.0000	H	-3.5301	-3.2277	0.0000
C	2.1431	1.6915	0.0000	C	-2.8588	1.0199	0.0000	H	-1.3863	-4.4876	0.0000
C	2.3953	-1.0987	0.0000	C	-3.5714	2.2015	0.0000	H	0.8097	-3.3246	0.0000
C	1.1371	-0.5230	0.0000	C	-4.9701	2.1341	0.0000	H	-3.0562	3.1672	0.0000
C	1.0015	0.9043	0.0000	C	-5.6288	0.9131	0.0000	H	-5.5500	3.0630	0.0000
C	-0.3045	1.5442	0.0000	C	-4.9170	-0.2930	0.0000	H	-6.7235	0.8875	0.0000
C	-0.0622	-1.3439	0.0000	H	6.9687	-0.5230	0.0000	H	-5.4406	-1.2541	0.0000
C	-2.5779	-2.6882	0.0000	H	6.7451	1.9429	0.0000				

Table 3.232: Table of thermodynamic data as a function of temperature for Dibenz[*e,k*]acephenanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.985	415.509	415.509	∞
100	99.583	337.225	724.648	-38.742	438.827	477.898	-249.623
200	193.453	433.387	555.058	-24.334	426.553	521.846	-136.289
250	248.803	482.448	535.606	-13.290	420.722	546.344	-114.150
298.15	303.104	530.922	530.922	0.000	415.509	571.024	-100.039
300	305.169	532.803	530.928	0.563	415.317	571.987	-99.590
350	359.515	583.967	534.844	17.193	410.500	598.491	-89.318
400	409.965	635.317	544.195	36.449	406.309	625.632	-81.697
450	455.685	686.291	557.157	58.110	402.672	653.270	-75.828
500	496.561	736.460	572.587	81.936	399.511	681.305	-71.174
600	565.125	833.302	608.041	135.157	394.357	738.174	-64.262
700	619.377	924.649	646.814	194.485	390.567	795.800	-59.382
800	662.913	1010.300	686.955	258.676	387.983	853.871	-55.751
900	698.412	1090.498	727.386	326.800	386.450	912.196	-52.941
1000	727.750	1165.649	767.495	398.153	385.823	970.654	-50.701
1100	752.257	1236.194	806.931	472.190	385.930	1029.146	-48.869
1200	772.903	1302.559	845.496	548.476	386.647	1087.584	-47.340
1300	790.421	1365.135	883.084	626.666	387.813	1145.954	-46.044
1400	805.378	1424.273	919.648	706.475	389.315	1204.223	-44.929
1500	818.223	1480.288	955.173	787.671	391.079	1262.378	-43.959
1600	829.311	1533.457	989.669	870.061	392.992	1320.401	-43.106
1700	838.933	1584.029	1023.156	953.485	394.989	1378.280	-42.349
1800	847.322	1632.224	1055.665	1037.807	397.005	1436.098	-41.674
1900	854.670	1678.238	1087.230	1122.914	399.013	1493.757	-41.065
2000	861.135	1722.244	1117.889	1208.711	400.964	1551.335	-40.516
2100	866.846	1764.400	1147.678	1295.116	402.791	1608.805	-40.016
2200	871.913	1804.845	1176.637	1382.059	404.493	1666.194	-39.560
2300	876.424	1843.705	1204.800	1469.480	406.065	1723.507	-39.141
2400	880.456	1881.092	1232.205	1557.328	407.445	1780.714	-38.755
2500	884.072	1917.108	1258.885	1645.558	408.645	1837.966	-38.401
2600	887.326	1951.847	1284.874	1734.130	409.632	1895.072	-38.072
2700	890.262	1985.391	1310.201	1823.012	410.410	1952.207	-37.767
2800	892.921	2017.816	1334.897	1912.174	410.956	2009.338	-37.484
2900	895.335	2049.193	1358.990	2001.588	411.245	2066.405	-37.219
3000	897.533	2079.584	1382.506	2091.233	411.315	2123.490	-36.972
3100	899.538	2109.047	1405.470	2181.088	411.098	2180.510	-36.741
3200	901.373	2137.636	1427.906	2271.135	410.631	2237.605	-36.524
3300	903.057	2165.398	1449.835	2361.358	409.897	2294.754	-36.322
3400	904.604	2192.381	1471.280	2451.742	408.873	2351.852	-36.131
3500	906.029	2218.624	1492.259	2542.275	407.563	2408.969	-35.951
3600	907.344	2244.166	1512.793	2632.944	405.986	2466.204	-35.783
3700	908.560	2269.043	1532.897	2723.740	404.114	2523.503	-35.625
3800	909.688	2293.288	1552.590	2814.653	401.924	2580.802	-35.475
3900	910.734	2316.931	1571.886	2905.675	399.452	2638.118	-35.333
4000	911.706	2340.001	1590.802	2996.798	396.685	2695.623	-35.201
4100	912.612	2362.525	1609.351	3088.014	393.590	2753.136	-35.075
4200	913.457	2384.527	1627.547	3179.318	390.193	2810.720	-34.956
4300	914.246	2406.031	1645.402	3270.704	386.481	2868.310	-34.842
4400	914.985	2427.057	1662.929	3362.166	382.462	2926.070	-34.736
4500	915.676	2447.627	1680.139	3453.699	378.148	2983.975	-34.636
4600	916.325	2467.760	1697.043	3545.299	373.495	3041.987	-34.542
4700	916.935	2487.473	1713.651	3636.963	368.514	3100.002	-34.452
4800	917.508	2506.784	1729.975	3728.685	363.248	3158.220	-34.368
4900	918.047	2525.708	1746.022	3820.463	357.630	3216.432	-34.287
5000	918.556	2544.260	1761.801	3912.294	351.743	3274.927	-34.212

3.233. Naphtho[1,2-*k*]fluoranthene



Other names: Acenaphtho[1,2-*b*]phenanthrene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 238-04-0

Point Group: C_s

Length: 15.37 Å

Width: 9.446 Å

Breadth: 3.888 Å

L/B Ratio: 1.627

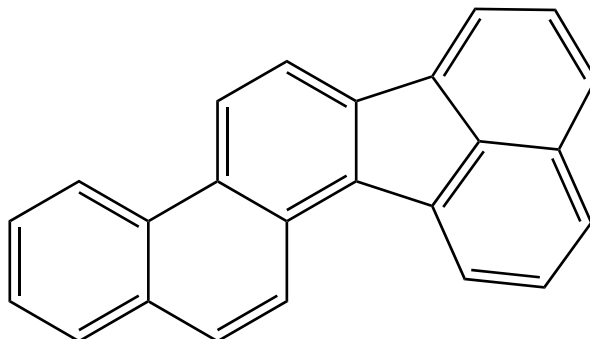
Cartesian coordinates:

C	5.7981	-0.9836	0.0000	C	-0.9701	0.9616	0.0000	H	2.6833	-2.3896	0.0000
C	5.4487	0.3464	0.0000	C	-1.8840	-1.2161	0.0000	H	5.0934	-3.0313	0.0000
C	3.4733	-1.6231	0.0000	C	-4.6009	-1.9623	0.0000	H	4.5154	2.8636	0.0000
C	4.8020	-1.9759	0.0000	C	-3.5921	-2.8956	0.0000	H	2.1271	3.5382	0.0000
C	3.0889	-0.2631	0.0000	C	-2.2130	-2.5430	0.0000	H	-0.2347	2.9814	0.0000
C	4.0878	0.7268	0.0000	C	-2.9380	-0.2511	0.0000	H	0.9443	-1.9168	0.0000
C	3.7174	2.1123	0.0000	C	-2.4335	1.0860	0.0000	H	-5.6517	-2.2707	0.0000
C	2.4128	2.4799	0.0000	C	-3.3263	2.1214	0.0000	H	-3.8459	-3.9615	0.0000
C	1.6983	0.1291	0.0000	C	-4.7160	1.8131	0.0000	H	-1.4483	-3.3258	0.0000
C	1.3689	1.4958	0.0000	C	-5.1945	0.5247	0.0000	H	-2.9975	3.1652	0.0000
C	0.0106	1.9135	0.0000	C	-4.2888	-0.5735	0.0000	H	-5.4239	2.6494	0.0000
C	0.6697	-0.8510	0.0000	H	6.8523	-1.2793	0.0000	H	-6.2713	0.3251	0.0000
C	-0.6347	-0.4441	0.0000	H	6.2201	1.1249	0.0000				

Table 3.233: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*k*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.672	412.653	412.653	∞
100	98.135	336.321	721.221	-38.490	436.223	475.385	-248.310
200	192.215	431.464	552.601	-24.227	423.804	519.481	-135.672
250	247.735	480.269	533.229	-13.240	417.915	544.082	-113.677
298.15	302.095	528.561	528.561	0.000	412.653	568.871	-99.662
300	304.161	530.436	528.567	0.561	412.459	569.839	-99.216
350	358.524	581.446	532.471	17.141	407.592	596.465	-89.016
400	408.986	632.664	541.795	36.348	403.352	623.736	-81.450
450	454.727	683.524	554.723	57.961	399.666	651.509	-75.624
500	495.636	733.594	570.114	81.740	396.459	679.685	-71.005
600	564.286	830.275	605.489	134.872	391.216	736.850	-64.147
700	618.631	921.499	644.185	194.120	387.346	794.785	-59.306
800	662.255	1007.056	684.255	258.242	384.693	853.175	-55.705
900	697.832	1087.181	724.621	326.304	383.097	911.829	-52.920
1000	727.237	1162.275	764.672	397.603	382.416	970.621	-50.699
1100	751.801	1232.774	804.056	471.590	382.475	1029.453	-48.884
1200	772.497	1299.102	842.573	547.834	383.148	1088.235	-47.369
1300	790.057	1361.647	880.120	625.986	384.277	1146.952	-46.084
1400	805.052	1420.759	916.645	705.760	385.743	1205.572	-44.979
1500	817.928	1476.752	952.136	786.925	387.476	1264.079	-44.018
1600	829.044	1529.904	986.599	869.287	389.361	1322.456	-43.173
1700	838.690	1580.460	1020.057	952.685	391.333	1380.692	-42.423
1800	847.100	1628.642	1052.540	1036.984	393.326	1438.867	-41.754
1900	854.467	1674.644	1084.081	1122.070	395.313	1496.885	-41.151
2000	860.948	1718.641	1114.717	1207.848	397.244	1554.822	-40.607
2100	866.675	1760.788	1144.486	1294.235	399.053	1612.653	-40.112
2200	871.754	1801.225	1173.425	1381.161	400.738	1670.404	-39.660
2300	876.277	1840.078	1201.571	1468.567	402.295	1728.080	-39.245
2400	880.320	1877.459	1228.959	1556.401	403.662	1785.649	-38.863
2500	883.945	1913.470	1255.623	1644.617	404.848	1843.265	-38.512
2600	887.208	1948.204	1281.597	1733.178	405.823	1900.735	-38.185
2700	890.152	1981.744	1306.911	1822.048	406.589	1958.235	-37.884
2800	892.818	2014.165	1331.594	1911.199	407.125	2015.730	-37.603
2900	895.238	2045.538	1355.675	2000.604	407.404	2073.163	-37.341
3000	897.441	2075.926	1379.180	2090.239	407.464	2130.613	-37.097
3100	899.453	2105.386	1402.133	2180.086	407.239	2187.999	-36.867
3200	901.293	2133.972	1424.558	2270.124	406.763	2245.460	-36.653
3300	902.980	2161.733	1446.478	2360.339	406.022	2302.975	-36.452
3400	904.531	2188.713	1467.914	2450.716	404.991	2360.441	-36.263
3500	905.960	2214.954	1488.885	2541.241	403.673	2417.924	-36.085
3600	907.279	2240.494	1509.410	2631.904	402.089	2475.527	-35.918
3700	908.499	2265.369	1529.506	2722.694	400.211	2533.192	-35.762
3800	909.629	2289.613	1549.191	2813.601	398.015	2590.859	-35.613
3900	910.678	2313.255	1568.481	2904.617	395.538	2648.542	-35.473
4000	911.653	2336.323	1587.390	2995.734	392.765	2706.416	-35.341
4100	912.561	2358.846	1605.932	3086.945	389.665	2764.296	-35.217
4200	913.409	2380.847	1624.122	3178.244	386.263	2822.249	-35.099
4300	914.200	2402.349	1641.971	3269.625	382.546	2880.206	-34.987
4400	914.940	2423.374	1659.492	3361.083	378.523	2938.335	-34.882
4500	915.634	2443.944	1676.697	3452.612	374.205	2996.608	-34.783
4600	916.285	2464.075	1693.595	3544.208	369.547	3054.988	-34.690
4700	916.896	2483.788	1710.199	3635.867	364.562	3113.372	-34.601
4800	917.470	2503.098	1726.517	3727.586	359.292	3171.959	-34.517
4900	918.011	2522.021	1742.560	3819.360	353.670	3230.539	-34.437
5000	918.521	2540.572	1758.335	3911.187	347.780	3289.403	-34.363

3.234. Naphtho[2,1-j]fluoranthene



Formula: C₂₄H₁₄
Mass: 302.368 g/mol
Point Group: C_s

Length: 15.59 Å
Width: 9.564 Å
Breadth: 3.887 Å
L/B Ratio: 1.630

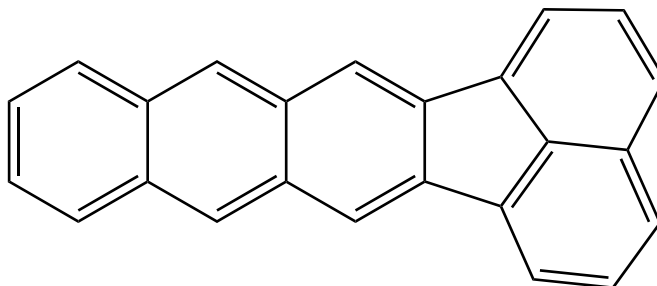
Cartesian coordinates:

C	5.1535	0.3706	0.0000	C	-1.2424	2.0566	0.0000	H	3.2429	3.2260	0.0000
C	4.8115	1.7018	0.0000	C	-0.8583	-0.3605	0.0000	H	1.0131	-3.0561	0.0000
C	3.4616	2.1537	0.0000	C	-1.7458	0.7420	0.0000	H	3.3371	-3.9486	0.0000
C	4.1384	-0.6276	0.0000	C	-2.7160	-1.9251	0.0000	H	5.3140	-2.4601	0.0000
C	1.8668	-2.3635	0.0000	C	-1.3827	-1.6990	0.0000	H	0.5001	3.3394	0.0000
C	3.1990	-2.8617	0.0000	C	-3.6483	-0.8305	0.0000	H	-1.9616	2.8904	0.0000
C	4.3021	-2.0413	0.0000	C	-3.1738	0.4930	0.0000	H	-3.1157	-2.9457	0.0000
C	2.8294	-0.1651	0.0000	C	-4.1062	1.5518	0.0000	H	-0.6616	-2.5313	0.0000
C	2.4663	1.2165	0.0000	C	-5.4592	1.2969	0.0000	H	-3.7272	2.5853	0.0000
C	1.6754	-1.0086	0.0000	C	-5.9289	-0.0258	0.0000	H	-6.1761	2.1245	0.0000
C	0.5183	-0.0994	0.0000	C	-5.0374	-1.0754	0.0000	H	-7.0071	-0.2159	0.0000
C	0.9972	1.2357	0.0000	H	6.2038	0.0603	0.0000	H	-5.3981	-2.1104	0.0000
C	0.1177	2.3137	0.0000	H	5.6029	2.4596	0.0000				

Table 3.234: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*j*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-45.289	426.110	426.110	∞
100	100.324	342.882	731.450	-38.857	449.313	487.818	-254.805
200	194.051	439.408	561.391	-24.396	437.091	531.180	-138.727
250	249.454	488.611	541.891	-13.320	431.292	555.373	-116.036
298.15	303.713	537.196	537.196	0.000	426.110	579.753	-101.568
300	305.776	539.082	537.202	0.564	425.919	580.705	-101.108
350	360.046	590.333	541.126	17.223	421.130	606.893	-90.572
400	410.421	641.749	550.492	36.503	416.964	633.714	-82.753
450	456.076	692.773	563.472	58.186	413.347	661.029	-76.729
500	496.894	742.980	578.921	82.030	410.205	688.739	-71.951
600	565.355	839.874	614.410	135.278	405.079	744.953	-64.853
700	619.515	931.249	653.214	194.624	401.307	801.921	-59.839
800	662.971	1016.913	693.381	258.825	398.733	859.331	-56.107
900	698.405	1097.114	733.834	326.952	397.202	916.994	-53.220
1000	727.693	1172.261	773.959	398.302	396.572	974.790	-50.917
1100	752.164	1242.800	813.408	472.331	396.671	1032.621	-49.034
1200	772.785	1309.156	851.983	548.607	397.377	1090.400	-47.463
1300	790.288	1371.721	889.580	626.784	398.532	1148.110	-46.131
1400	805.236	1430.849	926.150	706.579	400.019	1205.721	-44.985
1500	818.076	1486.854	961.680	787.761	401.769	1263.219	-43.988
1600	829.165	1540.014	996.179	870.136	403.667	1320.586	-43.112
1700	838.788	1590.577	1029.668	953.545	405.650	1377.810	-42.334
1800	847.180	1638.764	1062.179	1037.853	407.652	1434.973	-41.641
1900	854.533	1684.770	1093.745	1122.946	409.645	1491.979	-41.017
2000	861.003	1728.769	1124.404	1208.730	411.583	1548.904	-40.452
2100	866.720	1770.919	1154.194	1295.122	413.397	1605.722	-39.939
2200	871.792	1811.358	1183.153	1382.053	415.086	1662.459	-39.471
2300	876.309	1850.213	1211.316	1469.462	416.647	1719.122	-39.042
2400	880.347	1887.595	1238.721	1557.298	418.016	1775.677	-38.646
2500	883.968	1923.607	1265.400	1645.517	419.205	1832.280	-38.283
2600	887.226	1958.342	1291.388	1734.080	420.182	1888.736	-37.944
2700	890.168	1991.882	1316.714	1822.952	420.950	1945.222	-37.632
2800	892.831	2024.304	1341.410	1912.104	421.487	2001.703	-37.341
2900	895.250	2055.678	1365.502	2001.510	421.767	2058.122	-37.070
3000	897.451	2086.066	1389.017	2091.147	421.829	2114.559	-36.817
3100	899.461	2115.526	1411.980	2180.994	421.604	2170.930	-36.579
3200	901.300	2144.112	1434.414	2271.033	421.129	2227.378	-36.357
3300	902.986	2171.873	1456.343	2361.249	420.389	2283.879	-36.150
3400	904.537	2198.853	1477.787	2451.626	419.358	2340.330	-35.954
3500	905.965	2225.094	1498.765	2542.152	418.041	2396.800	-35.770
3600	907.283	2250.635	1519.297	2632.815	416.457	2453.388	-35.597
3700	908.502	2275.510	1539.401	2723.605	414.579	2510.040	-35.435
3800	909.632	2299.754	1559.092	2814.513	412.384	2566.692	-35.281
3900	910.680	2323.395	1578.388	2905.529	409.907	2623.362	-35.135
4000	911.655	2346.464	1597.303	2996.646	407.134	2680.221	-34.999
4100	912.563	2368.987	1615.851	3087.858	404.035	2737.087	-34.870
4200	913.410	2390.988	1634.045	3179.157	400.633	2794.025	-34.748
4300	914.201	2412.490	1651.900	3270.538	396.916	2850.969	-34.632
4400	914.941	2433.516	1669.426	3361.996	392.892	2908.084	-34.523
4500	915.635	2454.085	1686.635	3453.525	388.574	2965.343	-34.420
4600	916.285	2474.217	1703.538	3545.121	383.917	3022.708	-34.323
4700	916.896	2493.929	1720.146	3636.780	378.932	3080.078	-34.231
4800	917.471	2513.239	1736.468	3728.499	373.662	3137.651	-34.144
4900	918.011	2532.162	1752.515	3820.273	368.040	3195.217	-34.061
5000	918.521	2550.714	1768.294	3912.100	362.150	3253.067	-33.984

3.235. Naphtho[2,3-*k*]fluoranthene



Other names: Acenaphth[1,2-*b*]anthracene
Naphtho(2',3':8,9)fluoranthene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 207-18-1

Point Group: C_{2v}

Length: 15.98 Å

Width: 9.194 Å

Breadth: 3.884 Å

L/B Ratio: 1.739

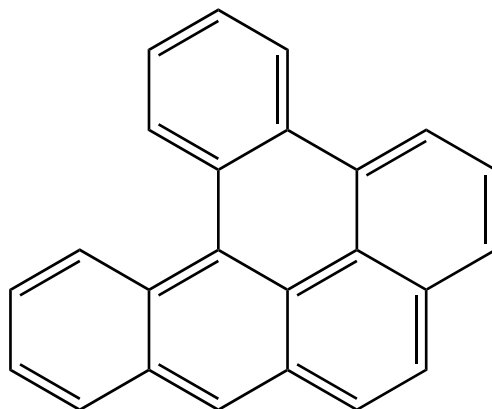
Cartesian coordinates:

C	-6.3267	0.3881	0.0000	C	0.9975	-0.6820	0.0000	H	-4.9812	-2.7581	0.0000
C	-6.2538	-1.0334	0.0000	C	2.2938	1.3034	0.0000	H	-5.2372	2.2339	0.0000
C	-5.0473	-1.6642	0.0000	C	5.1005	1.5413	0.0000	H	-2.5288	-2.6326	0.0000
C	-5.1911	1.1390	0.0000	C	4.2795	2.6434	0.0000	H	-2.7848	2.3599	0.0000
C	-3.9056	0.5099	0.0000	C	2.8596	2.5482	0.0000	H	-0.0794	-2.5344	0.0000
C	-3.8330	-0.9069	0.0000	C	4.5398	0.2330	0.0000	H	-0.3383	2.5128	0.0000
C	-2.5819	-1.5368	0.0000	C	3.1524	0.1617	0.0000	H	6.1900	1.6521	0.0000
C	-2.7256	1.2644	0.0000	C	2.4153	-1.0620	0.0000	H	4.7239	3.6448	0.0000
C	-1.4812	0.6380	0.0000	C	3.1058	-2.2422	0.0000	H	2.2501	3.4571	0.0000
C	-1.4082	-0.7864	0.0000	C	4.5281	-2.1912	0.0000	H	2.5928	-3.2088	0.0000
C	-0.1245	-1.4397	0.0000	C	5.2317	-1.0109	0.0000	H	5.0727	-3.1419	0.0000
C	-0.2711	1.4192	0.0000	H	-7.3127	0.8640	0.0000	H	6.3268	-1.0092	0.0000
C	0.9224	0.7803	0.0000	H	-7.1860	-1.6077	0.0000				

Table 3.235: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*k*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-44.845	427.615	427.615	∞
100	98.349	330.902	717.503	-38.660	451.015	490.718	-256.320
200	193.112	426.410	548.115	-24.341	438.652	535.340	-139.814
250	248.914	475.448	528.652	-13.301	432.816	560.188	-117.042
298.15	303.445	523.963	523.963	0.000	427.615	585.204	-102.523
300	305.515	525.847	523.969	0.563	427.423	586.181	-102.061
350	359.944	577.071	527.890	17.213	422.626	613.031	-91.488
400	410.394	628.479	537.252	36.491	418.457	640.515	-83.641
450	456.078	679.502	550.229	58.173	414.840	668.493	-77.595
500	496.908	729.710	565.675	82.017	411.699	696.867	-72.800
600	565.390	826.608	601.161	135.268	406.574	754.408	-65.676
700	619.587	917.991	639.963	194.620	402.808	812.702	-60.643
800	663.091	1003.668	680.130	258.830	400.243	871.437	-56.898
900	698.570	1083.885	720.584	326.971	398.727	930.425	-53.999
1000	727.895	1159.052	760.713	398.340	398.115	989.542	-51.687
1100	752.392	1229.611	800.166	472.390	398.236	1048.693	-49.797
1200	773.030	1295.988	838.746	548.690	398.966	1107.789	-48.220
1300	790.541	1358.573	876.349	626.892	400.145	1166.815	-46.882
1400	805.491	1417.720	912.925	706.713	401.658	1225.741	-45.732
1500	818.329	1473.742	948.462	787.920	403.433	1284.551	-44.731
1600	829.411	1526.918	982.968	870.320	405.356	1343.228	-43.851
1700	839.026	1577.496	1016.465	953.753	407.363	1401.761	-43.070
1800	847.409	1625.696	1048.983	1038.084	409.388	1460.231	-42.374
1900	854.752	1671.715	1080.556	1123.200	411.404	1518.543	-41.747
2000	861.211	1715.725	1111.223	1209.005	413.363	1576.773	-41.180
2100	866.918	1757.885	1141.019	1295.418	415.198	1634.895	-40.665
2200	871.980	1798.333	1169.984	1382.368	416.907	1692.935	-40.195
2300	876.488	1837.195	1198.154	1469.795	418.485	1750.900	-39.763
2400	880.516	1874.585	1225.565	1557.649	419.872	1808.757	-39.366
2500	884.128	1910.604	1252.250	1645.885	421.078	1866.660	-39.001
2600	887.379	1945.345	1278.244	1734.463	422.070	1924.416	-38.661
2700	890.312	1978.891	1303.576	1823.350	422.853	1982.201	-38.347
2800	892.968	2011.318	1328.276	1912.516	423.404	2039.981	-38.056
2900	895.380	2042.696	1352.374	2001.935	423.697	2097.699	-37.783
3000	897.575	2073.088	1375.894	2091.585	423.772	2155.433	-37.529
3100	899.578	2102.553	1398.861	2181.444	423.559	2213.102	-37.290
3200	901.411	2131.143	1421.301	2271.495	423.096	2270.847	-37.067
3300	903.093	2158.907	1443.234	2361.721	422.366	2328.645	-36.859
3400	904.638	2185.890	1464.682	2452.109	421.346	2386.393	-36.662
3500	906.061	2212.134	1485.664	2542.644	420.039	2444.159	-36.476
3600	907.375	2237.677	1506.200	2633.317	418.464	2502.043	-36.303
3700	908.590	2262.555	1526.307	2724.116	416.595	2559.990	-36.140
3800	909.716	2286.801	1546.003	2815.032	414.408	2617.938	-35.985
3900	910.761	2310.445	1565.302	2906.057	411.940	2675.902	-35.839
4000	911.732	2333.516	1584.220	2997.182	409.175	2734.057	-35.702
4100	912.637	2356.040	1602.771	3088.401	406.083	2792.218	-35.573
4200	913.481	2378.042	1620.969	3179.707	402.688	2850.451	-35.450
4300	914.269	2399.546	1638.827	3271.095	398.978	2908.688	-35.333
4400	915.006	2420.574	1656.356	3362.559	394.961	2967.098	-35.223
4500	915.697	2441.144	1673.568	3454.095	390.650	3025.651	-35.120
4600	916.345	2461.277	1690.474	3545.697	385.998	3084.310	-35.023
4700	916.954	2480.991	1707.084	3637.363	381.020	3142.974	-34.930
4800	917.526	2500.302	1723.409	3729.087	375.755	3201.840	-34.842
4900	918.065	2519.226	1739.458	3820.867	370.139	3260.700	-34.759
5000	918.573	2537.779	1755.239	3912.699	364.254	3319.844	-34.681

3.236. Dibenzo[*def,p*]chrysene



Other names: Dibenzo[*a,l*]pyrene
 2,3:4,5-Dibenzopyrene
 3,4:8,9-Dibenzopyrene
 4,5,6,7-Dibenzopyrene
 1,2:9,10-Dibenzopyrene
 1,2:3,4-Dibenzopyrene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 191-30-0
Point Group: C₁

Length: 13.73 Å
Width: 11.60 Å
Breadth: 4.850 Å
L/B Ratio: 1.184

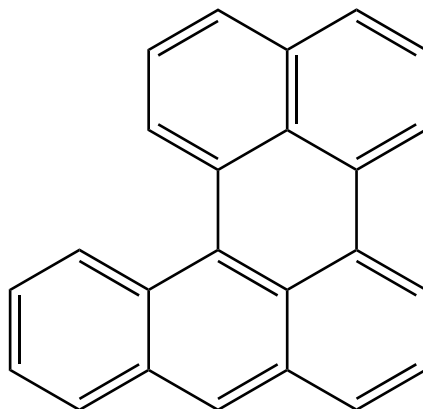
Cartesian coordinates:

C	4.3325	-0.8387	-0.5970	C	-3.5628	-0.5572	-0.4209	H	4.4282	2.4608	0.2388
C	4.8716	0.4344	-0.3017	C	0.6698	-0.2381	0.0535	H	2.5949	-2.0595	-0.7458
C	4.0337	1.4590	0.0330	C	-0.1531	0.8955	0.1179	H	2.2173	3.3463	0.5054
C	2.9883	-1.0650	-0.4949	C	-1.5848	0.7853	-0.0110	H	0.0077	4.3270	0.5505
C	2.0824	-0.0412	-0.0914	C	-2.1852	-0.4767	-0.1887	H	-2.4507	4.1075	0.2807
C	2.6259	1.2513	0.1057	C	0.0292	-1.5476	0.1384	H	-4.3958	2.7340	-0.2238
C	1.7774	2.3564	0.3307	C	-1.3619	-1.6647	-0.0567	H	-5.4225	0.5078	-0.6295
C	0.4099	2.1984	0.2766	C	-1.9689	-2.9344	-0.0444	H	-4.0213	-1.5463	-0.5719
C	-0.4582	3.3509	0.3714	C	-1.2366	-4.0696	0.2321	H	-3.0491	-3.0047	-0.2452
C	-1.7924	3.2329	0.2270	C	0.1227	-3.9506	0.5325	H	-1.7169	-5.0532	0.2369
C	-2.3966	1.9423	-0.0047	C	0.7362	-2.7147	0.4890	H	0.7001	-4.8401	0.8054
C	-3.7718	1.8331	-0.2235	H	5.0063	-1.6410	-0.9157	H	1.8031	-2.6488	0.7425
C	-4.3462	0.5878	-0.4449	H	5.9538	0.5874	-0.3603				

Table 3.236: Table of thermodynamic data as a function of temperature for Dibenzo[def,p]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-44.219	403.294	403.294	∞
100	95.343	329.555	712.316	-38.276	427.078	466.916	-243.887
200	191.459	423.539	544.380	-24.168	414.504	511.766	-133.657
250	247.156	472.200	525.052	-13.213	408.583	536.767	-112.149
298.15	301.554	520.393	520.393	0.000	403.294	561.948	-98.449
300	303.621	522.265	520.399	0.560	403.099	562.931	-98.013
350	358.020	573.194	524.297	17.114	398.206	589.967	-88.046
400	408.539	624.348	533.607	36.297	393.942	617.652	-80.655
450	454.348	675.160	546.518	57.889	390.235	645.842	-74.966
500	495.320	725.193	561.892	81.651	387.011	674.438	-70.457
600	564.063	821.825	597.232	134.756	381.741	732.445	-63.764
700	618.449	913.019	635.898	193.985	377.852	791.227	-59.041
800	662.083	998.553	675.942	258.089	375.181	850.467	-55.529
900	697.654	1078.657	716.286	326.134	373.568	909.971	-52.812
1000	727.050	1153.732	756.317	397.414	372.868	969.617	-50.647
1100	751.607	1224.213	795.683	471.383	372.908	1029.304	-48.877
1200	772.299	1290.523	834.184	547.607	373.562	1088.943	-47.399
1300	789.859	1353.052	871.715	625.738	374.671	1148.518	-46.147
1400	804.855	1412.150	908.227	705.494	376.118	1207.998	-45.070
1500	817.736	1468.130	943.704	786.639	377.831	1267.367	-44.133
1600	828.858	1521.269	978.155	868.982	379.697	1326.607	-43.308
1700	838.511	1571.815	1011.602	952.362	381.651	1385.707	-42.577
1800	846.930	1619.986	1044.074	1036.643	383.626	1444.747	-41.925
1900	854.304	1665.979	1075.604	1121.713	385.596	1503.631	-41.337
2000	860.794	1709.968	1106.231	1207.475	387.512	1562.436	-40.806
2100	866.528	1752.108	1135.990	1293.847	389.306	1621.134	-40.323
2200	871.615	1792.539	1164.921	1380.759	390.977	1679.753	-39.882
2300	876.146	1831.385	1193.059	1468.151	392.520	1738.298	-39.477
2400	880.195	1868.761	1220.439	1555.972	393.874	1796.737	-39.104
2500	883.827	1904.767	1247.097	1644.176	395.048	1855.223	-38.762
2600	887.096	1939.496	1273.063	1732.725	396.011	1913.563	-38.443
2700	890.046	1973.032	1298.371	1821.585	396.767	1971.934	-38.149
2800	892.717	2005.450	1323.048	1910.725	397.292	2030.301	-37.875
2900	895.143	2036.819	1347.123	2000.120	397.561	2088.605	-37.619
3000	897.351	2067.204	1370.622	2089.747	397.613	2146.928	-37.381
3100	899.367	2096.661	1393.570	2179.584	397.378	2205.186	-37.156
3200	901.211	2125.244	1415.990	2269.614	396.894	2263.520	-36.947
3300	902.902	2153.003	1437.905	2359.821	396.145	2321.908	-36.752
3400	904.457	2179.980	1459.336	2450.190	395.106	2380.246	-36.567
3500	905.890	2206.219	1480.302	2540.708	393.782	2438.603	-36.393
3600	907.212	2231.758	1500.823	2631.364	392.191	2497.079	-36.231
3700	908.435	2256.631	1520.916	2722.147	390.306	2555.619	-36.078
3800	909.568	2280.873	1540.597	2813.048	388.103	2614.159	-35.933
3900	910.619	2304.513	1559.883	2904.058	385.620	2672.717	-35.796
4000	911.597	2327.580	1578.788	2995.170	382.842	2731.464	-35.669
4100	912.508	2350.101	1597.327	3086.375	379.737	2790.219	-35.547
4200	913.357	2372.101	1615.513	3177.669	376.329	2849.046	-35.432
4300	914.151	2393.602	1633.359	3269.045	372.607	2907.878	-35.323
4400	914.893	2414.627	1650.877	3360.498	368.579	2966.882	-35.221
4500	915.588	2435.195	1668.079	3452.022	364.256	3026.030	-35.125
4600	916.241	2455.326	1684.975	3543.614	359.594	3085.285	-35.034
4700	916.853	2475.037	1701.576	3635.269	354.605	3144.544	-34.947
4800	917.430	2494.346	1717.891	3726.983	349.330	3204.005	-34.866
4900	917.972	2513.268	1733.931	3818.754	343.705	3263.461	-34.788
5000	918.484	2531.819	1749.704	3910.577	337.811	3323.200	-34.717

3.237. Benzo[*a*]perylene



Other names: 1,2-Benzoperylene
1,2-Benzperylene
Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 191-85-5
Point Group: C₁

Length: 13.73 Å
Width: 11.59 Å
Breadth: 4.993 Å
L/B Ratio: 1.185

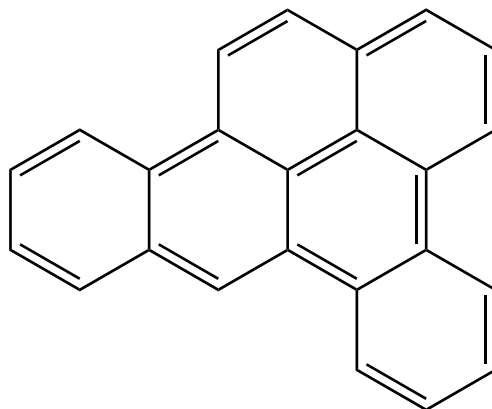
Cartesian coordinates:

C	4.3828	0.1289	0.0610	C	1.1461	-3.5123	-0.2961	H	-3.6017	3.5546	-0.3249
C	3.0192	-0.3042	-0.0330	C	-0.5207	1.1217	-0.2232	H	-3.5414	-2.2939	0.5887
C	1.9597	0.6400	0.0911	C	-1.8428	0.6228	0.0063	H	-5.4364	-0.6922	0.7987
C	2.3325	1.9807	0.4363	C	-2.0874	-0.7689	0.1828	H	-5.0756	1.7308	0.3547
C	3.6339	2.3580	0.5602	C	-0.3897	2.4360	-0.6259	H	1.9862	-4.2055	-0.4181
C	4.6833	1.4238	0.3429	C	-1.4955	3.3092	-0.6772	H	-0.3564	-5.0381	-0.2683
C	0.6206	0.2102	-0.0761	C	-2.7437	2.8732	-0.3271	H	-2.2283	-3.4364	0.0685
C	0.3573	-1.1777	-0.1046	C	-2.9418	1.5087	0.0101	H	3.5651	-2.3712	-0.3617
C	1.4241	-2.1107	-0.2131	C	-3.3634	-1.2151	0.4607	H	1.5402	2.7191	0.6216
C	2.7427	-1.6571	-0.2289	C	-4.4394	-0.3113	0.5543	H	3.8919	3.3858	0.8361
C	-0.9783	-1.6997	0.0061	C	-4.2401	1.0227	0.3174	H	5.7219	1.7608	0.4205
C	-1.2019	-3.0530	-0.0400	H	-1.3350	4.3474	-0.9866	H	5.1752	-0.6135	-0.0891
C	-0.1332	-3.9677	-0.2125	H	0.5942	2.8406	-0.9007				

Table 3.237: Table of thermodynamic data as a function of temperature for Benzo[*a*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-44.399	437.960	437.960	∞
100	95.717	329.766	714.224	-38.446	461.574	501.391	-261.895
200	192.359	424.185	545.546	-24.272	449.066	546.199	-142.650
250	248.228	473.067	526.136	-13.267	443.195	571.162	-119.335
298.15	302.729	521.459	521.459	0.000	437.960	596.296	-104.466
300	304.799	523.338	521.464	0.562	437.767	597.277	-103.993
350	359.246	574.453	525.377	17.177	432.935	624.255	-93.163
400	409.769	625.771	534.720	36.421	428.732	651.873	-85.124
450	455.550	676.727	547.673	58.074	425.086	679.988	-78.929
500	496.475	726.883	563.094	81.894	421.921	708.502	-74.015
600	565.095	823.716	598.533	135.110	416.761	766.330	-66.714
700	619.356	915.060	637.295	194.435	412.968	824.914	-61.555
800	662.875	1000.707	677.427	258.624	410.382	883.945	-57.714
900	698.347	1080.898	717.851	326.743	408.843	943.229	-54.742
1000	727.659	1156.041	757.953	398.088	408.208	1002.647	-52.372
1100	752.144	1226.577	797.382	472.114	408.305	1062.100	-50.434
1200	772.775	1292.931	835.941	548.389	409.010	1121.501	-48.817
1300	790.283	1355.497	873.523	626.565	410.163	1180.834	-47.445
1400	805.236	1414.624	910.081	706.360	411.650	1240.068	-46.267
1500	818.078	1470.629	945.601	787.542	413.400	1299.188	-45.241
1600	829.168	1523.789	980.090	869.918	415.299	1358.177	-44.339
1700	838.792	1574.353	1013.572	953.327	417.282	1417.024	-43.539
1800	847.185	1622.540	1046.076	1037.635	419.284	1475.809	-42.826
1900	854.538	1668.546	1077.636	1122.729	421.278	1534.437	-42.184
2000	861.008	1712.546	1108.289	1208.513	423.216	1592.985	-41.604
2100	866.725	1754.696	1138.074	1294.906	425.031	1651.425	-41.076
2200	871.797	1795.135	1167.027	1381.837	426.721	1709.785	-40.595
2300	876.314	1833.990	1195.187	1469.247	428.282	1768.069	-40.153
2400	880.351	1871.372	1222.587	1557.084	429.652	1826.248	-39.746
2500	883.972	1907.384	1249.263	1645.303	430.841	1884.472	-39.373
2600	887.231	1942.119	1275.248	1733.866	431.818	1942.550	-39.026
2700	890.172	1975.660	1300.571	1822.739	432.587	2000.659	-38.704
2800	892.835	2008.082	1325.264	1911.891	433.124	2058.762	-38.406
2900	895.253	2039.456	1349.353	2001.297	433.404	2116.804	-38.127
3000	897.455	2069.844	1372.866	2090.935	433.467	2174.863	-37.867
3100	899.464	2099.304	1395.826	2180.782	433.242	2232.856	-37.623
3200	901.303	2127.891	1418.259	2270.822	432.768	2290.926	-37.395
3300	902.989	2155.651	1440.185	2361.038	432.028	2349.049	-37.182
3400	904.540	2182.632	1461.627	2451.415	430.997	2407.123	-36.980
3500	905.968	2208.873	1482.604	2541.941	429.680	2465.214	-36.791
3600	907.286	2234.414	1503.134	2632.605	428.097	2523.425	-36.613
3700	908.505	2259.289	1523.236	2723.395	426.219	2581.698	-36.446
3800	909.634	2283.532	1542.926	2814.303	424.024	2639.973	-36.288
3900	910.683	2307.174	1562.221	2905.319	421.547	2698.265	-36.138
4000	911.657	2330.243	1581.134	2996.437	418.775	2756.746	-35.999
4100	912.565	2352.766	1599.681	3087.649	415.676	2815.234	-35.866
4200	913.412	2374.767	1617.874	3178.948	412.274	2873.795	-35.740
4300	914.203	2396.269	1635.727	3270.329	408.557	2932.360	-35.620
4400	914.943	2417.295	1653.252	3361.787	404.534	2991.097	-35.508
4500	915.636	2437.864	1670.460	3453.316	400.216	3049.978	-35.402
4600	916.287	2457.996	1687.363	3544.913	395.559	3108.966	-35.303
4700	916.898	2477.708	1703.970	3636.572	390.574	3167.958	-35.207
4800	917.472	2497.018	1720.291	3728.291	385.304	3227.153	-35.118
4900	918.013	2515.941	1736.336	3820.066	379.683	3286.341	-35.032
5000	918.523	2534.493	1752.114	3911.893	373.793	3345.813	-34.953

3.238. Naphtho[1,2,3,4-*def*]chrysene



Other names: Dibenzo[*a,e*]pyrene
1,2:4,5-Dibenzopyrene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 192-65-4
Point Group: C_s

Length: 13.81 Å
Width: 11.14 Å
Breadth: 3.886 Å
L/B Ratio: 1.239

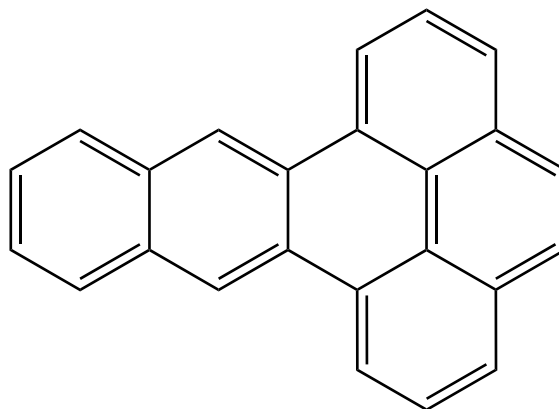
Cartesian coordinates:

C	5.0589	-0.1434	0.0000	C	-0.9320	-2.6294	0.0000	H	3.6590	2.9686	0.0000
C	4.9666	1.2647	0.0000	C	0.3535	-3.2592	0.0000	H	3.9808	-2.0101	0.0000
C	3.7397	1.8756	0.0000	C	1.4875	-2.5138	0.0000	H	1.2241	2.8277	0.0000
C	3.9234	-0.9110	0.0000	C	1.4346	-1.0832	0.0000	H	-4.4169	-0.8947	0.0000
C	2.6408	-0.3060	0.0000	C	0.1916	-0.4424	0.0000	H	-4.2614	-3.3742	0.0000
C	2.5518	1.0992	0.0000	C	-2.3657	0.8612	0.0000	H	-2.0400	-4.4932	0.0000
C	1.2767	1.7269	0.0000	C	-1.1921	1.6342	0.0000	H	0.3990	-4.3542	0.0000
C	0.1186	0.9894	0.0000	C	-1.2960	3.0337	0.0000	H	2.4810	-2.9881	0.0000
C	-2.2862	-0.5958	0.0000	C	-2.5324	3.6554	0.0000	H	-0.3730	3.6338	0.0000
C	-3.4296	-1.3818	0.0000	C	-3.6968	2.8875	0.0000	H	-2.5973	4.7482	0.0000
C	-3.3423	-2.7790	0.0000	C	-3.6117	1.5063	0.0000	H	-4.6758	3.3775	0.0000
C	-2.1127	-3.3998	0.0000	H	6.0470	-0.6150	0.0000	H	-4.5256	0.8925	0.0000
C	-1.0123	-1.2221	0.0000	H	5.8848	1.8611	0.0000				

Table 3.238: Table of thermodynamic data as a function of temperature for Naphtho[1,2,3,4-*def*]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-44.597	373.888	373.888	∞
100	97.367	337.705	721.439	-38.373	397.575	436.598	-228.051
200	191.798	432.516	553.296	-24.156	385.110	480.577	-125.511
250	246.999	481.195	533.984	-13.197	379.193	505.128	-105.539
298.15	301.070	529.331	529.331	0.000	373.888	529.877	-92.830
300	303.126	531.200	529.337	0.559	373.692	530.843	-92.426
350	357.311	582.035	533.228	17.083	368.769	557.435	-83.191
400	407.707	633.086	542.521	36.226	364.465	584.680	-76.350
450	453.457	683.796	555.406	57.775	360.716	612.437	-71.088
500	494.414	733.733	570.750	81.492	357.446	640.603	-66.922
600	563.195	830.203	606.023	134.508	352.087	697.764	-60.745
700	617.658	921.269	644.620	193.654	348.115	755.715	-56.391
800	661.374	1006.702	684.599	257.683	345.369	814.135	-53.156
900	697.021	1086.728	724.883	325.661	343.689	872.829	-50.657
1000	726.486	1161.739	764.858	396.881	342.929	931.670	-48.664
1100	751.103	1232.169	804.172	470.797	342.916	990.559	-47.037
1200	771.847	1298.438	842.627	546.973	343.522	1049.405	-45.678
1300	789.453	1360.933	880.116	625.062	344.588	1108.191	-44.527
1400	804.489	1420.003	916.590	704.778	345.996	1166.884	-43.536
1500	817.405	1475.958	952.032	785.889	347.675	1225.469	-42.674
1600	828.558	1529.077	986.452	868.200	349.510	1283.927	-41.915
1700	838.237	1579.605	1019.869	951.551	351.435	1342.247	-41.241
1800	846.679	1627.762	1052.314	1035.807	353.384	1400.509	-40.641
1900	854.075	1673.742	1083.819	1120.852	355.329	1458.616	-40.099
2000	860.583	1717.719	1114.423	1206.592	357.223	1516.645	-39.610
2100	866.333	1759.849	1144.162	1292.944	358.997	1574.569	-39.164
2200	871.435	1800.271	1173.072	1379.837	360.649	1632.414	-38.758
2300	875.979	1839.110	1201.192	1467.212	362.175	1690.186	-38.385
2400	880.040	1876.479	1228.555	1555.017	363.513	1747.853	-38.040
2500	883.683	1912.479	1255.196	1643.206	364.672	1805.568	-37.724
2600	886.961	1947.203	1281.148	1731.741	365.621	1863.137	-37.430
2700	889.920	1980.733	1306.441	1820.588	366.364	1920.737	-37.158
2800	892.600	2013.147	1331.105	1909.716	366.877	1978.334	-36.906
2900	895.032	2044.512	1355.168	1999.100	367.135	2035.869	-36.669
3000	897.247	2074.893	1378.655	2088.715	367.175	2093.423	-36.449
3100	899.269	2104.347	1401.592	2178.543	366.931	2150.912	-36.242
3200	901.119	2132.927	1424.001	2268.563	366.437	2208.478	-36.049
3300	902.815	2160.683	1445.907	2358.761	365.679	2266.098	-35.869
3400	904.375	2187.658	1467.328	2449.122	364.632	2323.668	-35.698
3500	905.812	2213.894	1488.285	2539.632	363.299	2381.257	-35.538
3600	907.138	2239.431	1508.797	2630.280	361.701	2438.966	-35.388
3700	908.364	2264.302	1528.882	2721.056	359.808	2496.738	-35.247
3800	909.501	2288.542	1548.555	2811.950	357.599	2554.512	-35.113
3900	910.555	2312.181	1567.834	2902.954	355.110	2612.302	-34.987
4000	911.536	2335.246	1586.732	2994.059	352.325	2670.283	-34.870
4100	912.450	2357.766	1605.264	3085.259	349.214	2728.271	-34.758
4200	913.302	2379.764	1623.444	3176.547	345.801	2786.332	-34.652
4300	914.098	2401.264	1641.283	3267.917	342.073	2844.398	-34.552
4400	914.842	2422.287	1658.795	3359.365	338.040	2902.635	-34.458
4500	915.540	2442.854	1675.991	3450.884	333.712	2961.017	-34.370
4600	916.194	2462.984	1692.882	3542.471	329.045	3019.506	-34.287
4700	916.809	2482.695	1709.477	3634.122	324.052	3077.999	-34.207
4800	917.387	2502.003	1725.788	3725.832	318.773	3136.695	-34.133
4900	917.931	2520.924	1741.823	3817.598	313.143	3195.385	-34.063
5000	918.444	2539.474	1757.591	3909.417	307.245	3254.359	-33.997

3.239. Dibenzo[*de,qr*]naphthacene



Other names: Dibenzo[*de,qr*]tetracene
Naphtho-(2'3':4,5)pyrene
Naphtho[2,3-*e*]pyrene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 193-09-9
Point Group: C_{2v}

Length: 14.27 Å
Width: 11.13 Å
Breadth: 3.886 Å
L/B Ratio: 1.282

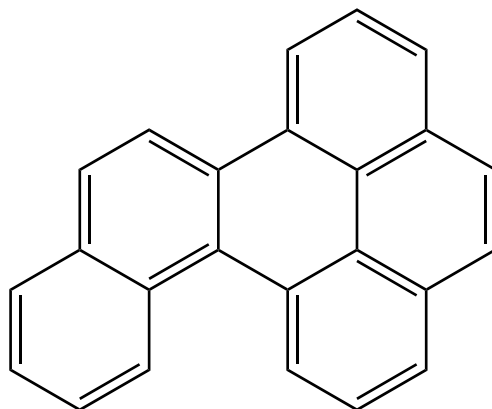
Cartesian coordinates:

C	-5.4916	0.6974	0.0000	C	3.0710	1.4214	0.0000	H	-4.2986	-2.5066	0.0000
C	-5.4887	-0.7200	0.0000	C	3.0716	2.8272	0.0000	H	-4.3089	2.4890	0.0000
C	-4.3098	-1.4109	0.0000	C	1.8767	3.5196	0.0000	H	-1.8317	-2.5007	0.0000
C	-4.3156	1.3932	0.0000	C	0.6613	2.8318	0.0000	H	-1.8420	2.4932	0.0000
C	-3.0719	0.6994	0.0000	C	0.6281	1.4413	0.0000	H	5.2499	-1.2308	0.0000
C	-3.0690	-0.7119	0.0000	C	3.0767	-1.4088	0.0000	H	5.2448	1.2523	0.0000
C	-1.8353	-1.3986	0.0000	C	1.8504	-0.7153	0.0000	H	4.0258	3.3661	0.0000
C	-1.8410	1.3910	0.0000	C	0.6340	-1.4387	0.0000	H	1.8757	4.6146	0.0000
C	-0.6373	0.7124	0.0000	C	0.6729	-2.8291	0.0000	H	-0.2873	3.3905	0.0000
C	-0.6344	-0.7150	0.0000	C	1.8911	-3.5119	0.0000	H	-0.2734	-3.3917	0.0000
C	4.3095	-0.6677	0.0000	C	3.0832	-2.8146	0.0000	H	1.8946	-4.6069	0.0000
C	4.3067	0.6854	0.0000	H	-6.4510	1.2251	0.0000	H	4.0396	-3.3495	0.0000
C	1.8475	0.7229	0.0000	H	-6.4459	-1.2516	0.0000				

Table 3.239: Table of thermodynamic data as a function of temperature for Dibenzo[de,qr]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-44.294	372.511	372.511	∞
100	95.798	327.870	710.318	-38.245	396.326	436.333	-227.912
200	191.229	421.892	542.569	-24.135	383.754	481.346	-125.712
250	246.821	470.490	523.268	-13.194	377.819	506.430	-105.811
298.15	301.115	518.616	518.616	0.000	372.511	531.695	-93.149
300	303.178	520.485	518.621	0.559	372.315	532.681	-92.746
350	357.473	571.337	522.514	17.088	367.398	559.809	-83.545
400	407.913	622.413	531.810	36.241	363.104	587.588	-76.730
450	453.674	673.148	544.701	57.801	359.365	615.877	-71.488
500	494.629	723.108	560.051	81.529	356.106	644.575	-67.337
600	563.402	819.616	595.340	134.566	350.768	702.797	-61.183
700	617.867	910.714	633.954	193.732	346.817	761.805	-56.845
800	661.591	996.176	673.948	257.782	344.092	821.279	-53.623
900	697.248	1076.228	714.247	325.783	342.434	881.024	-51.132
1000	726.719	1151.263	754.237	397.026	341.698	940.915	-49.147
1100	751.338	1221.716	793.566	470.965	341.707	1000.850	-47.525
1200	772.080	1288.005	832.034	547.165	342.337	1060.740	-46.172
1300	789.680	1350.518	869.536	625.276	343.426	1120.568	-45.024
1400	804.709	1409.604	906.022	705.015	344.857	1180.302	-44.037
1500	817.616	1465.575	941.476	786.148	346.557	1239.926	-43.177
1600	828.759	1518.707	975.907	868.480	348.412	1299.422	-42.421
1700	838.429	1569.247	1009.335	951.850	350.357	1358.778	-41.749
1800	846.860	1617.414	1041.790	1036.124	352.325	1418.075	-41.151
1900	854.246	1663.404	1073.305	1121.188	354.288	1477.217	-40.611
2000	860.744	1707.390	1103.918	1206.944	356.198	1536.279	-40.123
2100	866.486	1749.527	1133.665	1293.311	357.988	1595.236	-39.678
2200	871.579	1789.956	1162.583	1380.219	359.655	1654.113	-39.273
2300	876.114	1828.801	1190.711	1467.608	361.195	1712.916	-38.901
2400	880.168	1866.175	1218.081	1555.426	362.546	1771.613	-38.557
2500	883.803	1902.181	1244.729	1643.628	363.717	1830.358	-38.242
2600	887.075	1936.909	1270.688	1732.175	364.678	1888.957	-37.949
2700	890.028	1970.444	1295.987	1821.032	365.432	1947.586	-37.678
2800	892.701	2002.861	1320.657	1910.171	365.955	2006.212	-37.426
2900	895.128	2034.230	1344.725	1999.564	366.223	2064.775	-37.190
3000	897.338	2064.614	1368.218	2089.189	366.273	2123.357	-36.970
3100	899.355	2094.071	1391.160	2179.026	366.037	2181.874	-36.764
3200	901.201	2122.654	1413.574	2269.055	365.552	2240.467	-36.571
3300	902.893	2150.412	1435.484	2359.261	364.802	2299.114	-36.391
3400	904.449	2177.389	1456.910	2449.629	363.762	2357.712	-36.221
3500	905.882	2203.628	1477.872	2540.146	362.437	2416.328	-36.061
3600	907.205	2229.166	1498.388	2630.802	360.845	2475.063	-35.911
3700	908.428	2254.040	1518.476	2721.584	358.959	2533.861	-35.771
3800	909.562	2278.281	1538.154	2812.484	356.756	2592.661	-35.638
3900	910.614	2301.921	1557.436	2903.494	354.273	2651.478	-35.512
4000	911.592	2324.988	1576.337	2994.604	351.494	2710.484	-35.395
4100	912.503	2347.509	1594.873	3085.810	348.388	2769.498	-35.283
4200	913.353	2369.509	1613.056	3177.103	344.980	2828.585	-35.178
4300	914.147	2391.010	1630.898	3268.478	341.258	2887.676	-35.078
4400	914.889	2412.034	1648.414	3359.931	337.229	2946.939	-34.984
4500	915.585	2432.602	1665.612	3451.455	332.906	3006.346	-34.896
4600	916.238	2452.733	1682.505	3543.046	328.244	3065.860	-34.813
4700	916.850	2472.444	1699.104	3634.701	323.254	3125.378	-34.734
4800	917.427	2491.753	1715.417	3726.415	317.979	3185.100	-34.660
4900	917.970	2510.676	1731.454	3818.185	312.354	3244.814	-34.589
5000	918.481	2529.226	1747.225	3910.008	306.459	3304.813	-34.524

3.240. Naphtho[8,1,2-*ghi*]chrysene



Other names: Naphtho[1,2-*e*]pyrene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 35699-67-3

Point Group: C₁

Length: 13.78 Å

Width: 10.42 Å

Breadth: 4.871 Å

L/B Ratio: 1.323

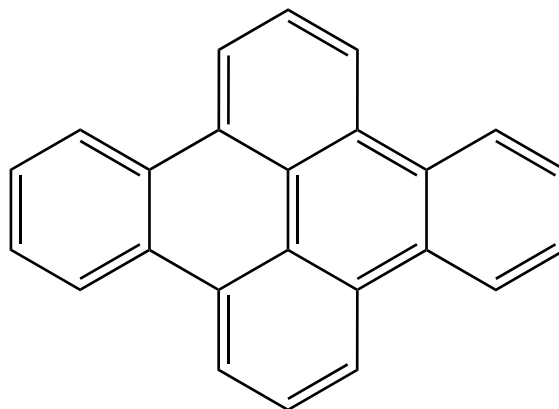
Cartesian coordinates:

C	5.1623	-0.2925	0.3374	C	0.4160	-2.4083	-0.4755	H	2.3594	-2.1702	0.7852
C	4.5899	0.8916	-0.0445	C	-1.0391	1.5529	-0.0756	H	4.7980	-2.3199	1.0068
C	2.9770	-1.3015	0.5195	C	-1.5755	2.8417	-0.0538	H	3.2634	3.1350	-0.6175
C	4.3386	-1.3918	0.6506	C	-2.9408	3.0456	0.1249	H	0.7994	3.4259	-0.5184
C	2.3474	-0.1102	0.0700	C	-3.7989	1.9685	0.2731	H	-2.5228	-4.1137	-0.2255
C	3.1800	1.0098	-0.1466	C	-1.9098	0.4498	0.0632	H	-0.1140	-4.4799	-0.7316
C	2.6041	2.2822	-0.4197	C	-3.2953	0.6619	0.2330	H	1.4724	-2.6147	-0.6951
C	1.2536	2.4323	-0.3848	C	-4.1745	-0.4726	0.3375	H	-0.9073	3.7073	-0.1762
C	0.9198	0.0264	-0.0976	C	-3.6955	-1.7302	0.2100	H	-3.3359	4.0667	0.1471
C	0.3917	1.3139	-0.1914	C	-2.2932	-1.9705	-0.0120	H	-4.8733	2.1316	0.4140
C	0.0022	-1.1083	-0.1788	C	-1.3907	-0.8844	-0.0242	H	-5.2409	-0.2864	0.5090
C	-1.8231	-3.2706	-0.2384	H	6.2495	-0.3901	0.4185	H	-4.3628	-2.5978	0.2694
C	-0.4810	-3.4736	-0.5032	H	5.2112	1.7678	-0.2627				

Table 3.240: Table of thermodynamic data as a function of temperature for Naphtho[8,1,2-*ghi*]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-44.141	395.195	395.195	∞
100	94.859	330.373	712.278	-38.190	419.065	458.821	-239.659
200	191.007	423.973	544.662	-24.138	406.435	503.611	-131.527
250	246.856	472.550	525.355	-13.201	400.496	528.592	-110.441
298.15	301.356	520.700	520.700	0.000	395.195	553.757	-97.014
300	303.426	522.570	520.706	0.559	395.000	554.740	-96.587
350	357.892	573.475	524.601	17.106	390.099	581.762	-86.821
400	408.456	624.615	533.908	36.283	385.829	609.433	-79.582
450	454.295	675.419	546.814	57.872	382.119	637.610	-74.010
500	495.289	725.447	562.184	81.632	378.893	666.193	-69.595
600	564.057	822.076	597.517	134.735	373.622	724.174	-63.044
700	618.456	913.271	636.178	193.964	369.733	782.931	-58.422
800	662.094	998.805	676.219	258.069	367.062	842.146	-54.985
900	697.666	1078.911	716.561	326.115	365.450	901.625	-52.328
1000	727.062	1153.987	756.590	397.397	364.752	961.245	-50.209
1100	751.618	1224.469	795.954	471.367	364.793	1020.907	-48.478
1200	772.308	1290.781	834.454	547.592	365.448	1080.520	-47.033
1300	789.867	1353.310	871.984	625.724	366.557	1140.070	-45.808
1400	804.862	1412.409	908.495	705.480	368.005	1199.524	-44.754
1500	817.742	1468.389	943.971	786.626	369.719	1258.867	-43.837
1600	828.864	1521.528	978.422	868.970	371.586	1318.081	-43.030
1700	838.516	1572.074	1011.868	952.350	373.540	1377.155	-42.314
1800	846.934	1620.246	1044.340	1036.632	375.516	1436.169	-41.676
1900	854.308	1666.240	1075.870	1121.702	377.486	1495.027	-41.100
2000	860.797	1710.228	1106.496	1207.464	379.402	1553.806	-40.580
2100	866.531	1752.368	1136.256	1293.836	381.196	1612.478	-40.107
2200	871.618	1792.799	1165.186	1380.749	382.868	1671.071	-39.675
2300	876.148	1831.646	1193.324	1468.141	384.411	1729.590	-39.279
2400	880.197	1869.021	1220.704	1555.962	385.765	1788.003	-38.914
2500	883.829	1905.028	1247.361	1644.167	386.940	1846.463	-38.579
2600	887.097	1939.757	1273.328	1732.716	387.903	1904.777	-38.267
2700	890.048	1973.293	1298.635	1821.576	388.659	1963.122	-37.978
2800	892.719	2005.711	1323.312	1910.716	389.184	2021.462	-37.710
2900	895.144	2037.080	1347.387	2000.111	389.453	2079.741	-37.459
3000	897.352	2067.465	1370.886	2089.738	389.505	2138.037	-37.226
3100	899.368	2096.922	1393.833	2179.575	389.270	2196.269	-37.006
3200	901.212	2125.506	1416.254	2269.606	388.787	2254.577	-36.801
3300	902.903	2153.264	1438.169	2359.813	388.038	2312.939	-36.610
3400	904.458	2180.241	1459.600	2450.182	386.999	2371.251	-36.429
3500	905.890	2206.480	1480.566	2540.700	385.674	2429.582	-36.259
3600	907.213	2232.019	1501.087	2631.356	384.083	2488.032	-36.100
3700	908.435	2256.892	1521.179	2722.139	382.198	2546.545	-35.950
3800	909.568	2281.134	1540.860	2813.040	379.996	2605.060	-35.808
3900	910.620	2304.774	1560.146	2904.050	377.513	2663.591	-35.674
4000	911.598	2327.842	1579.051	2995.162	374.735	2722.312	-35.549
4100	912.508	2350.363	1597.590	3086.367	371.630	2781.041	-35.430
4200	913.358	2372.362	1615.776	3177.661	368.222	2839.842	-35.318
4300	914.151	2393.863	1633.622	3269.037	364.500	2898.648	-35.211
4400	914.893	2414.888	1651.140	3360.490	360.472	2957.626	-35.111
4500	915.589	2435.456	1668.342	3452.014	356.149	3016.748	-35.017
4600	916.241	2455.587	1685.238	3543.606	351.487	3075.976	-34.928
4700	916.854	2475.298	1701.838	3635.261	346.498	3135.209	-34.843
4800	917.430	2494.607	1718.154	3726.976	341.224	3194.645	-34.764
4900	917.973	2513.530	1734.194	3818.746	335.598	3254.074	-34.688
5000	918.484	2532.080	1749.967	3910.569	329.704	3313.787	-34.618

3.241. Dibenzo[*fg,op*]naphthacene



Other names: Dibenzo[*e,l*]pyrene
4,5,9,10-Dibenzopyrene
1,2:6,7-Dibenzopyrene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 192-51-8
Point Group: D_{2h}

Length: 13.79 Å
Width: 10.41 Å
Breadth: 3.886 Å
L/B Ratio: 1.325

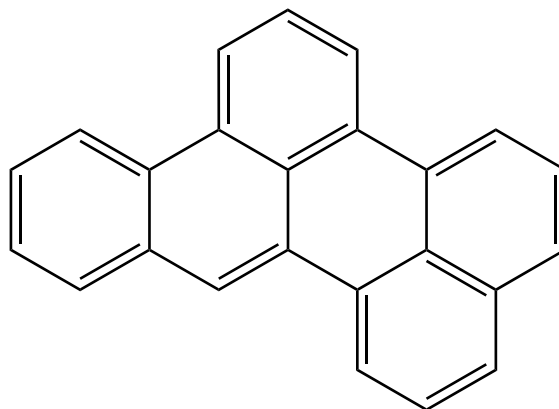
Cartesian coordinates:

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C	-4.9063	-0.6896	0.0000	C	0.0014	0.7218	0.0000	H	-3.6954	2.4954	0.0000
C	-3.7105	-1.3807	0.0000	C	-0.0014	-0.7217	0.0000	H	2.1633	3.3733	0.0000
C	-3.7053	1.3947	0.0000	C	1.2173	-1.4338	0.0000	H	0.0087	4.6174	0.0000
C	-2.4788	0.7069	0.0000	C	1.2227	1.4292	0.0000	H	-2.1506	3.3813	0.0000
C	-2.4814	-0.6976	0.0000	C	2.4814	0.6976	0.0000	H	-2.1634	-3.3732	0.0000
C	-1.2173	1.4338	0.0000	C	2.4788	-0.7070	0.0000	H	-0.0087	-4.6174	0.0000
C	1.2074	2.8275	0.0000	C	3.7053	-1.3947	0.0000	H	2.1505	-3.3815	0.0000
C	0.0066	3.5224	0.0000	C	4.9037	-0.7081	0.0000	H	3.6954	-2.4954	0.0000
C	-1.1967	2.8320	0.0000	C	4.9063	0.6896	0.0000	H	5.8517	-1.2555	0.0000
C	-1.2227	-1.4292	0.0000	C	3.7105	1.3807	0.0000	H	5.8564	1.2334	0.0000
C	-1.2074	-2.8275	0.0000	H	-5.8517	1.2555	0.0000	H	3.7048	2.4815	0.0000
C	-0.0067	-3.5224	0.0000	H	-5.8564	-1.2334	0.0000				

Table 3.241: Table of thermodynamic data as a function of temperature for Dibenzof[fg,op]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-44.636	372.908	372.908	∞
100	97.679	327.705	711.289	-38.358	396.610	436.633	-228.069
200	191.731	422.624	543.262	-24.128	384.159	481.604	-125.780
250	246.692	471.262	523.974	-13.178	378.232	506.651	-105.857
298.15	300.602	519.329	519.329	0.000	372.908	531.879	-93.181
300	302.655	521.194	519.334	0.558	372.711	532.864	-92.778
350	356.760	571.950	523.219	17.056	367.762	559.959	-83.568
400	407.137	622.926	532.497	36.171	363.431	587.710	-76.745
450	452.901	673.569	545.364	57.692	359.653	615.976	-71.499
500	493.883	723.449	560.686	81.381	356.356	644.655	-67.345
600	562.717	819.827	595.914	134.347	350.947	702.849	-61.187
700	617.216	910.822	634.468	193.447	346.929	761.841	-56.848
800	660.954	996.198	674.407	257.433	344.139	821.309	-53.625
900	696.618	1076.175	714.653	325.370	342.418	881.056	-51.134
1000	726.098	1151.144	754.593	396.551	341.619	940.955	-49.149
1100	750.730	1221.538	793.876	470.428	341.568	1000.905	-47.528
1200	771.490	1287.776	832.302	546.568	342.138	1060.816	-46.175
1300	789.113	1350.242	869.764	624.622	343.168	1120.669	-45.028
1400	804.167	1409.287	906.212	704.305	344.544	1180.433	-44.042
1500	817.101	1465.221	941.631	785.385	346.191	1240.090	-43.183
1600	828.272	1518.321	976.029	867.667	347.996	1299.623	-42.427
1700	837.969	1568.832	1009.426	950.990	349.894	1359.020	-41.757
1800	846.428	1616.974	1041.852	1035.220	351.817	1418.359	-41.159
1900	853.839	1662.941	1073.341	1120.241	353.738	1477.546	-40.620
2000	860.362	1706.907	1103.928	1205.958	355.609	1536.656	-40.132
2100	866.126	1749.026	1133.651	1292.288	357.361	1595.661	-39.689
2200	871.241	1789.439	1162.547	1379.161	358.994	1654.589	-39.284
2300	875.797	1828.269	1190.653	1466.518	360.501	1713.445	-38.913
2400	879.869	1865.631	1218.004	1554.305	361.821	1772.196	-38.570
2500	883.522	1901.624	1244.633	1642.477	362.964	1830.996	-38.256
2600	886.809	1936.342	1270.574	1730.997	363.897	1889.651	-37.963
2700	889.777	1969.867	1295.856	1819.829	364.625	1948.338	-37.692
2800	892.464	2002.275	1320.510	1908.943	365.124	2007.021	-37.441
2900	894.905	2033.636	1344.563	1998.313	365.369	2065.644	-37.205
3000	897.126	2064.013	1368.041	2087.916	365.397	2124.285	-36.986
3100	899.154	2093.463	1390.969	2177.732	365.140	2182.863	-36.780
3200	901.010	2122.040	1413.370	2267.742	364.636	2241.517	-36.588
3300	902.712	2149.792	1435.268	2357.929	363.867	2300.226	-36.409
3400	904.277	2176.764	1456.682	2448.280	362.810	2358.886	-36.239
3500	905.719	2202.998	1477.632	2538.780	361.468	2417.564	-36.079
3600	907.049	2228.532	1498.137	2629.420	359.860	2476.363	-35.930
3700	908.280	2253.401	1518.215	2720.187	357.959	2535.225	-35.790
3800	909.420	2277.638	1537.882	2811.072	355.742	2594.089	-35.658
3900	910.479	2301.275	1557.155	2902.068	353.244	2652.970	-35.532
4000	911.463	2324.339	1576.047	2993.166	350.452	2712.041	-35.415
4100	912.379	2346.856	1594.574	3084.358	347.334	2771.121	-35.304
4200	913.234	2368.853	1612.748	3175.640	343.914	2830.272	-35.199
4300	914.033	2390.351	1630.583	3267.003	340.180	2889.429	-35.099
4400	914.780	2411.373	1648.090	3358.444	336.140	2948.758	-35.005
4500	915.481	2431.939	1665.281	3449.958	331.806	3008.232	-34.918
4600	916.137	2452.067	1682.167	3541.539	327.133	3067.812	-34.835
4700	916.754	2471.777	1698.759	3633.184	322.134	3127.397	-34.756
4800	917.334	2491.084	1715.065	3724.889	316.850	3187.185	-34.683
4900	917.880	2510.004	1731.096	3816.650	311.215	3246.967	-34.612
5000	918.395	2528.553	1746.860	3908.464	305.312	3307.033	-34.548

3.242. Benzo[*b*]perylene



Other names: 2,3-Benzoperylene
Dibenzo[*de,op*]naphthacene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 197-70-6
Point Group: C_s

Length: 14.28 Å
Width: 10.33 Å
Breadth: 3.890 Å
L/B Ratio: 1.383

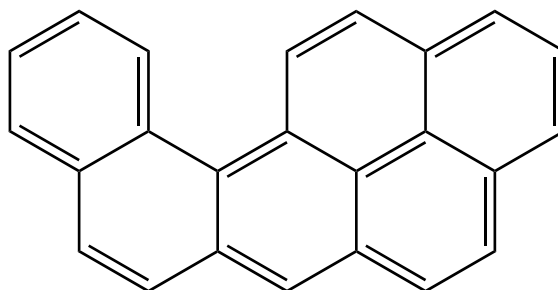
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C	3.6903	-2.0659	0.0000	C	-0.3935	2.9410	0.0000	H	-2.9221	3.0283	0.0000
C	2.6108	-1.1543	0.0000	C	-0.6491	1.5771	0.0000	H	-5.2513	2.1696	0.0000
C	2.8664	0.2273	0.0000	C	-1.1733	-1.2597	0.0000	H	-5.6887	-0.2800	0.0000
C	1.2604	-1.6258	0.0000	C	-2.2550	-0.3295	0.0000	H	3.0164	2.9100	0.0000
C	0.2024	-0.7625	0.0000	C	-3.5814	-0.8120	0.0000	H	1.0973	4.5044	0.0000
C	-2.0237	1.0779	0.0000	C	-3.8202	-2.2121	0.0000	H	-1.2381	3.6472	0.0000
C	-3.0997	1.9418	0.0000	C	-2.7695	-3.0894	0.0000	H	-4.8547	-2.5738	0.0000
C	-4.4218	1.4549	0.0000	C	-1.4432	-2.6128	0.0000	H	-2.9456	-4.1702	0.0000
C	-4.6635	0.1071	0.0000	H	5.8243	-2.3106	0.0000	H	-0.6088	-3.3311	0.0000
C	0.4343	0.6615	0.0000	H	6.2816	0.1297	0.0000				

Table 3.242: Table of thermodynamic data as a function of temperature for Benzo[*b*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-44.710	394.262	394.262	∞
100	97.652	341.208	725.747	-38.454	417.868	456.541	-238.467
200	192.227	436.278	557.271	-24.198	405.441	500.156	-130.625
250	247.433	485.055	537.926	-13.218	399.546	524.516	-109.589
298.15	301.492	533.266	533.266	0.000	394.262	549.077	-96.194
300	303.549	535.138	533.272	0.560	394.066	550.037	-95.768
350	357.713	586.037	537.168	17.104	389.164	576.430	-86.026
400	408.087	637.140	546.472	36.267	384.880	603.474	-78.804
450	453.814	687.893	559.371	57.835	381.149	631.026	-73.246
500	494.747	737.867	574.730	81.568	377.896	658.986	-68.842
600	563.486	834.393	610.033	134.616	372.569	715.731	-62.309
700	617.911	925.501	648.660	193.789	368.624	773.261	-57.700
800	661.597	1010.966	688.665	257.841	365.901	831.256	-54.274
900	697.219	1091.016	728.971	325.840	364.242	889.522	-51.625
1000	726.663	1166.047	768.968	397.080	363.501	947.934	-49.514
1100	751.262	1236.493	808.301	471.012	363.505	1006.391	-47.789
1200	771.990	1302.776	846.773	547.203	364.126	1064.804	-46.349
1300	789.582	1365.281	884.277	625.305	365.205	1123.155	-45.128
1400	804.606	1424.360	920.764	705.034	366.626	1181.414	-44.078
1500	817.511	1480.323	956.219	786.156	368.316	1239.562	-43.165
1600	828.655	1533.448	990.650	868.478	370.160	1297.584	-42.361
1700	838.326	1583.982	1024.077	951.838	372.095	1355.466	-41.648
1800	846.761	1632.144	1056.532	1036.102	374.052	1413.290	-41.012
1900	854.150	1678.128	1088.046	1121.155	376.006	1470.959	-40.439
2000	860.652	1722.109	1118.658	1206.902	377.907	1528.549	-39.921
2100	866.397	1764.242	1148.404	1293.260	379.687	1586.034	-39.450
2200	871.495	1804.667	1177.322	1380.160	381.346	1643.440	-39.019
2300	876.034	1843.509	1205.447	1467.541	382.878	1700.772	-38.625
2400	880.092	1880.880	1232.817	1555.351	384.221	1757.999	-38.261
2500	883.731	1916.882	1259.464	1643.545	385.385	1815.273	-37.927
2600	887.006	1951.607	1285.421	1732.085	386.339	1872.402	-37.616
2700	889.962	1985.139	1310.719	1820.936	387.086	1929.562	-37.329
2800	892.639	2017.554	1335.387	1910.068	387.603	1986.718	-37.062
2900	895.069	2048.921	1359.454	1999.455	387.864	2043.812	-36.812
3000	897.282	2079.304	1382.945	2089.075	387.908	2100.925	-36.580
3100	899.302	2108.759	1405.886	2178.905	387.667	2157.973	-36.361
3200	901.150	2137.340	1428.300	2268.929	387.177	2215.097	-36.157
3300	902.845	2165.096	1450.208	2359.130	386.422	2272.276	-35.966
3400	904.403	2192.072	1471.633	2449.494	385.377	2329.405	-35.786
3500	905.838	2218.310	1492.593	2540.007	384.047	2386.553	-35.617
3600	907.163	2243.847	1513.108	2630.657	382.451	2443.820	-35.458
3700	908.388	2268.719	1533.196	2721.436	380.561	2501.150	-35.309
3800	909.523	2292.959	1552.872	2812.332	378.355	2558.482	-35.168
3900	910.577	2316.598	1572.153	2903.338	375.867	2615.831	-35.034
4000	911.557	2339.665	1591.053	2994.445	373.085	2673.370	-34.910
4100	912.469	2362.185	1609.588	3085.647	369.976	2730.917	-34.792
4200	913.320	2384.183	1627.770	3176.937	366.564	2788.535	-34.680
4300	914.115	2405.684	1645.612	3268.309	362.839	2846.159	-34.573
4400	914.859	2426.707	1663.126	3359.758	358.807	2903.955	-34.474
4500	915.556	2447.275	1680.324	3451.279	354.481	2961.895	-34.380
4600	916.210	2467.405	1697.216	3542.868	349.816	3019.942	-34.292
4700	916.824	2487.116	1713.814	3634.520	344.824	3077.993	-34.207
4800	917.401	2506.424	1730.126	3726.231	339.546	3136.247	-34.129
4900	917.945	2525.346	1746.162	3817.999	333.918	3194.494	-34.053
5000	918.457	2543.896	1761.932	3909.819	328.021	3253.026	-33.983

3.243. Dibenzo[*c,mno*]chrysene



Other names: Naphtho[1,2-*a*]pyrene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 196-28-1

Point Group: C₁

Length: 14.40 Å

Width: 9.455 Å

Breadth: 4.792 Å

L/B Ratio: 1.523

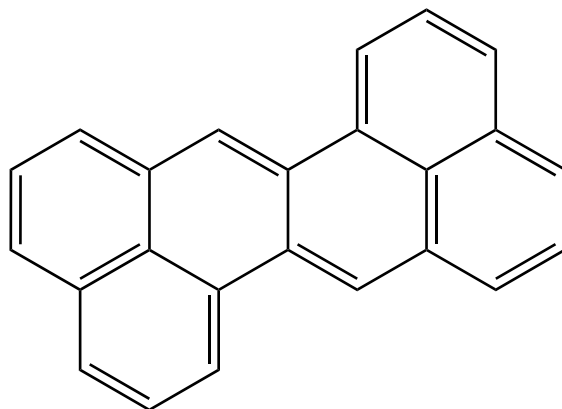
Cartesian coordinates:

C	-5.0921	-1.5865	-0.2660	C	3.5477	1.9652	-0.3347	H	-1.8007	-2.2740	-0.7599
C	-5.0001	-0.2588	0.0812	C	3.6475	0.5340	-0.1739	H	-4.0027	-3.3411	-0.9080
C	-2.6926	-1.6944	-0.4861	C	4.8820	-0.1112	-0.1975	H	-4.6292	2.3305	0.5629
C	-3.9262	-2.2988	-0.5809	C	4.9591	-1.4923	-0.0214	H	-2.4657	3.5409	0.3921
C	-2.5551	-0.3515	-0.0685	C	3.8133	-2.2407	0.1883	H	-0.1416	3.5710	-0.0092
C	-3.7427	0.3787	0.1482	C	-0.0037	-0.3347	0.1488	H	2.2705	3.6719	-0.3974
C	-3.6921	1.7954	0.3713	C	1.1805	0.4198	0.0188	H	4.4739	2.5311	-0.4872
C	-2.5129	2.4500	0.2927	C	2.4643	-0.2216	0.0185	H	5.7974	0.4709	-0.3537
C	-1.2708	0.3195	0.0632	C	2.5582	-1.6148	0.2139	H	5.9364	-1.9859	-0.0451
C	-1.2822	1.7300	0.1086	C	1.3526	-2.3501	0.4603	H	3.8790	-3.3245	0.3363
C	-0.0918	2.4747	0.0016	C	0.1445	-1.7375	0.4318	H	1.4349	-3.4198	0.6855
C	1.1283	1.8362	-0.0998	H	-6.0659	-2.0837	-0.3176	H	-0.7556	-2.3261	0.6562
C	2.3500	2.5840	-0.2889	H	-5.9048	0.3223	0.2945				

Table 3.243: Table of thermodynamic data as a function of temperature for Dibenzo[*c,mno*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-44.035	393.881	393.881	∞
100	94.137	330.036	711.291	-38.126	417.816	457.606	-239.024
200	190.724	423.219	543.871	-24.130	405.129	502.456	-131.225
250	246.805	471.761	524.566	-13.201	399.182	527.476	-110.208
298.15	301.395	519.911	519.911	0.000	393.881	552.679	-96.825
300	303.467	521.782	519.917	0.559	393.686	553.663	-96.399
350	357.939	572.694	523.813	17.108	388.788	580.724	-86.667
400	408.473	623.839	533.121	36.287	384.520	608.434	-79.452
450	454.276	674.642	546.028	57.876	380.810	636.650	-73.899
500	495.240	724.667	561.399	81.634	377.581	665.272	-69.499
600	563.981	821.284	596.732	134.731	372.304	723.332	-62.970
700	618.388	912.467	635.391	193.953	368.407	782.168	-58.365
800	662.052	997.994	675.430	258.052	365.731	841.464	-54.941
900	697.654	1078.097	715.769	326.095	364.117	901.024	-52.293
1000	727.077	1153.173	755.796	397.377	363.419	960.726	-50.182
1100	751.654	1223.657	795.158	471.350	363.462	1020.469	-48.457
1200	772.360	1289.973	833.657	547.579	364.122	1080.163	-47.017
1300	789.930	1352.507	871.186	625.717	365.237	1139.793	-45.797
1400	804.933	1411.611	907.697	705.480	366.691	1199.328	-44.747
1500	817.817	1467.596	943.174	786.633	368.413	1258.750	-43.833
1600	828.940	1520.740	977.625	868.985	370.287	1318.044	-43.029
1700	838.593	1571.291	1011.072	952.372	372.249	1377.196	-42.315
1800	847.009	1619.467	1043.544	1036.662	374.232	1436.288	-41.679
1900	854.382	1665.464	1075.075	1121.740	376.210	1495.224	-41.106
2000	860.869	1709.457	1105.702	1207.509	378.133	1554.080	-40.588
2100	866.600	1751.600	1135.463	1293.888	379.935	1612.829	-40.116
2200	871.684	1792.034	1164.394	1380.807	381.613	1671.499	-39.686
2300	876.212	1830.884	1192.533	1468.206	383.163	1730.094	-39.291
2400	880.258	1868.262	1219.915	1556.034	384.523	1788.583	-38.927
2500	883.887	1904.271	1246.573	1644.244	385.704	1847.119	-38.593
2600	887.153	1939.002	1272.541	1732.799	386.673	1905.508	-38.281
2700	890.101	1972.540	1297.850	1821.664	387.434	1963.928	-37.994
2800	892.769	2004.960	1322.528	1910.810	387.964	2022.344	-37.727
2900	895.192	2036.331	1346.604	2000.210	388.238	2080.698	-37.477
3000	897.398	2066.718	1370.104	2089.841	388.295	2139.069	-37.244
3100	899.411	2096.176	1393.053	2179.683	388.065	2197.375	-37.025
3200	901.254	2124.761	1415.474	2269.718	387.585	2255.758	-36.821
3300	902.943	2152.520	1437.390	2359.929	386.840	2314.194	-36.630
3400	904.496	2179.499	1458.822	2450.302	385.805	2372.581	-36.450
3500	905.927	2205.739	1479.790	2540.824	384.484	2430.986	-36.280
3600	907.247	2231.279	1500.311	2631.483	382.897	2489.510	-36.121
3700	908.469	2256.153	1520.405	2722.270	381.016	2548.097	-35.972
3800	909.600	2280.396	1540.087	2813.174	378.817	2606.685	-35.831
3900	910.650	2304.037	1559.373	2904.187	376.337	2665.290	-35.697
4000	911.627	2327.105	1578.280	2995.302	373.561	2724.085	-35.572
4100	912.536	2349.627	1596.819	3086.511	370.459	2782.888	-35.454
4200	913.384	2371.627	1615.006	3177.807	367.055	2841.762	-35.342
4300	914.177	2393.129	1632.853	3269.186	363.335	2900.642	-35.235
4400	914.918	2414.154	1650.372	3360.641	359.309	2959.693	-35.135
4500	915.613	2434.722	1667.574	3452.168	354.989	3018.888	-35.042
4600	916.264	2454.854	1684.471	3543.762	350.329	3078.190	-34.953
4700	916.876	2474.566	1701.072	3635.419	345.343	3137.496	-34.869
4800	917.451	2493.875	1717.389	3727.136	340.070	3197.005	-34.790
4900	917.993	2512.798	1733.429	3818.908	334.447	3256.507	-34.714
5000	918.504	2531.349	1749.203	3910.733	328.555	3316.294	-34.644

3.244. Dibenzo[*de,mn*]naphthacene



Other names: Zethrene
Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 214-63-1
Point Group: C_{2h}

Length: 14.29 Å
Width: 9.499 Å
Breadth: 3.888 Å
L/B Ratio: 1.504

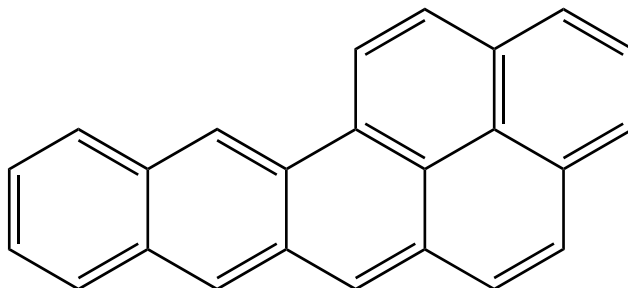
Cartesian coordinates:

C	4.5196	-1.9961	0.0000	C	3.9492	0.3566	0.0000	H	2.8596	-3.3904	0.0000
C	4.9151	-0.6827	0.0000	C	4.3364	1.7236	0.0000	H	0.4925	-2.7318	0.0000
C	3.1525	-2.3344	0.0000	C	3.3843	2.7076	0.0000	H	-0.4924	2.7318	0.0000
C	2.1892	-1.3448	0.0000	C	2.0130	2.3792	0.0000	H	-2.8595	3.3904	0.0000
C	0.7805	-1.6675	0.0000	C	1.5982	1.0629	0.0000	H	-5.2654	2.7979	0.0000
C	-0.1779	-0.7087	0.0000	C	-1.5983	-1.0630	0.0000	H	-5.9785	0.4182	0.0000
C	0.1779	0.7086	0.0000	C	-2.5781	-0.0260	0.0000	H	5.4034	1.9727	0.0000
C	-0.7804	1.6675	0.0000	C	-3.9492	-0.3566	0.0000	H	3.6760	3.7631	0.0000
C	-2.1892	1.3447	0.0000	C	-4.3364	-1.7235	0.0000	H	1.2600	3.1824	0.0000
C	-3.1524	2.3344	0.0000	C	-3.3844	-2.7076	0.0000	H	-5.4035	-1.9726	0.0000
C	-4.5195	1.9961	0.0000	C	-2.0131	-2.3792	0.0000	H	-3.6760	-3.7631	0.0000
C	-4.9150	0.6827	0.0000	H	5.2655	-2.7979	0.0000	H	-1.2601	-3.1824	0.0000
C	2.5781	0.0260	0.0000	H	5.9785	-0.4181	0.0000				

Table 3.244: Table of thermodynamic data as a function of temperature for Dibenzo[de,mn]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-44.528	431.306	431.306	∞
100	96.519	331.517	715.760	-38.424	454.942	494.584	-258.339
200	192.148	426.106	547.268	-24.232	442.452	539.201	-140.822
250	247.817	474.918	527.891	-13.243	436.565	564.070	-117.853
298.15	302.132	523.222	523.222	0.000	431.306	589.117	-103.209
300	304.195	525.097	523.228	0.561	431.112	590.094	-102.742
350	358.467	576.106	527.132	17.141	426.245	616.987	-92.078
400	408.856	627.311	536.455	36.342	422.000	644.525	-84.165
450	454.554	678.154	549.381	57.948	418.306	672.566	-78.068
500	495.441	728.203	564.768	81.717	415.090	701.012	-73.233
600	564.086	824.848	600.132	134.829	409.827	758.717	-66.051
700	618.442	916.043	638.816	194.059	405.938	817.196	-60.979
800	662.079	1001.575	678.873	258.162	403.266	876.134	-57.204
900	697.666	1081.680	719.228	326.207	401.653	935.336	-54.284
1000	727.080	1156.756	759.267	397.490	400.956	994.680	-51.956
1100	751.653	1227.241	798.639	471.462	400.999	1054.064	-50.052
1200	772.357	1293.556	837.147	547.691	401.659	1113.400	-48.464
1300	789.925	1356.090	874.683	625.829	402.773	1172.672	-47.118
1400	804.928	1415.194	911.200	705.591	404.228	1231.848	-45.960
1500	817.811	1471.178	946.682	786.744	405.948	1290.912	-44.953
1600	828.935	1524.322	981.138	869.095	407.822	1349.847	-44.067
1700	838.588	1574.873	1014.589	952.482	409.784	1408.641	-43.281
1800	847.005	1623.049	1047.065	1036.771	411.767	1467.375	-42.581
1900	854.378	1669.046	1078.599	1121.848	413.744	1525.953	-41.951
2000	860.865	1713.038	1109.229	1207.617	415.667	1584.451	-41.381
2100	866.596	1755.181	1138.993	1293.996	417.467	1642.842	-40.863
2200	871.681	1795.615	1167.926	1380.915	419.145	1701.154	-40.390
2300	876.209	1834.464	1196.067	1468.314	420.695	1759.391	-39.956
2400	880.255	1871.843	1223.451	1556.141	422.055	1817.521	-39.557
2500	883.885	1907.851	1250.111	1644.351	423.235	1875.699	-39.190
2600	887.150	1942.583	1276.081	1732.905	424.204	1933.731	-38.848
2700	890.098	1976.120	1301.390	1821.770	424.965	1991.793	-38.533
2800	892.767	2008.540	1326.070	1910.916	425.495	2049.851	-38.240
2900	895.190	2039.911	1350.147	2000.315	425.769	2107.846	-37.966
3000	897.396	2070.297	1373.649	2089.946	425.825	2165.860	-37.710
3100	899.410	2099.756	1396.599	2179.788	425.595	2223.808	-37.470
3200	901.252	2128.341	1419.021	2269.823	425.115	2281.833	-37.246
3300	902.942	2156.100	1440.938	2360.034	424.370	2339.911	-37.037
3400	904.495	2183.079	1462.371	2450.406	423.335	2397.940	-36.839
3500	905.925	2209.319	1483.339	2540.928	422.014	2455.987	-36.653
3600	907.246	2234.858	1503.862	2631.588	420.426	2514.152	-36.479
3700	908.467	2259.733	1523.956	2722.374	418.545	2572.382	-36.315
3800	909.599	2283.975	1543.639	2813.278	416.346	2630.612	-36.160
3900	910.649	2307.616	1562.926	2904.291	413.866	2688.859	-36.012
4000	911.626	2330.684	1581.833	2995.406	411.090	2747.296	-35.875
4100	912.535	2353.206	1600.373	3086.614	407.988	2805.741	-35.745
4200	913.383	2375.206	1618.561	3177.911	404.583	2864.257	-35.622
4300	914.176	2396.708	1636.408	3269.289	400.863	2922.779	-35.504
4400	914.917	2417.733	1653.928	3360.744	396.838	2981.472	-35.394
4500	915.612	2438.302	1671.130	3452.271	392.517	3040.309	-35.290
4600	916.263	2458.433	1688.028	3543.865	387.857	3099.253	-35.192
4700	916.875	2478.145	1704.630	3635.522	382.871	3158.201	-35.099
4800	917.451	2497.455	1720.946	3727.239	377.598	3217.352	-35.011
4900	917.992	2516.377	1736.987	3819.011	371.975	3276.497	-34.927
5000	918.503	2534.928	1752.761	3910.836	366.083	3335.925	-34.849

3.245. Naphtho[2,1,8-*gra*]naphthacene



Other names: Naphtho[2,3-*a*]pyrene
 Naphtho[2,3-*b*]pyrene
 Naphtho[2'.3',1.2]pyrene
 Naphtho[8,1,2-*cde*]naphthacene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 196-42-9
Point Group: C_s

Length: 16.09 Å
Width: 9.541 Å
Breadth: 3.886 Å
L/B Ratio: 1.687

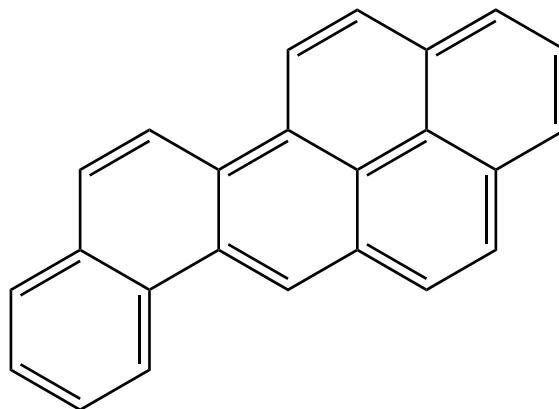
Cartesian coordinates:

C	5.7638	-1.2075	0.0000	C	-3.4649	2.2246	0.0000	H	5.2484	2.1759	0.0000
C	6.0486	0.1881	0.0000	C	-3.8073	0.8172	0.0000	H	4.2485	-2.7227	0.0000
C	5.0389	1.1002	0.0000	C	-5.1269	0.3919	0.0000	H	2.8391	2.6649	0.0000
C	4.4773	-1.6510	0.0000	C	-5.4288	-0.9766	0.0000	H	1.8307	-2.2322	0.0000
C	3.3889	-0.7206	0.0000	C	-4.4235	-1.9196	0.0000	H	0.4631	3.1690	0.0000
C	3.6726	0.6708	0.0000	C	-0.3713	-0.6711	0.0000	H	-1.9280	3.6987	0.0000
C	2.6194	1.5900	0.0000	C	-1.3923	0.2774	0.0000	H	-4.2887	2.9478	0.0000
C	2.0599	-1.1543	0.0000	C	-2.7600	-0.1423	0.0000	H	-5.9400	1.1266	0.0000
C	1.0061	-0.2401	0.0000	C	-3.0720	-1.5170	0.0000	H	-6.4772	-1.2932	0.0000
C	1.2924	1.1540	0.0000	C	-2.0063	-2.4703	0.0000	H	-4.6636	-2.9888	0.0000
C	0.2182	2.0994	0.0000	C	-0.7096	-2.0598	0.0000	H	-2.2586	-3.5367	0.0000
C	-1.0843	1.6837	0.0000	H	6.5999	-1.9145	0.0000	H	0.1177	-2.7862	0.0000
C	-2.1814	2.6321	0.0000	H	7.0949	0.5108	0.0000				

Table 3.245: Table of thermodynamic data as a function of temperature for Naphtho[2,1,8-*qra*]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-44.157	386.402	386.402	∞
100	94.821	331.880	713.823	-38.194	410.267	449.873	-234.985
200	191.052	425.436	546.173	-24.147	397.632	494.515	-129.151
250	246.978	474.034	526.858	-13.206	391.697	519.423	-108.525
298.15	301.418	522.202	522.202	0.000	386.402	544.516	-95.395
300	303.484	524.072	522.207	0.560	386.206	545.496	-94.977
350	357.807	574.976	526.103	17.105	381.305	572.442	-85.431
400	408.215	626.094	535.408	36.274	377.027	600.039	-78.355
450	453.926	676.862	548.310	57.848	373.302	628.143	-72.911
500	494.834	726.846	563.673	81.587	370.054	656.655	-68.599
600	563.543	823.385	598.984	134.641	364.734	714.501	-62.202
700	617.983	914.503	637.617	193.820	360.795	773.131	-57.691
800	661.706	999.979	677.628	257.881	358.081	832.225	-54.338
900	697.370	1080.045	717.941	325.894	356.435	891.589	-51.745
1000	726.850	1155.094	757.944	397.150	355.711	951.098	-49.679
1100	751.476	1225.559	797.285	471.102	355.735	1010.649	-47.991
1200	772.222	1291.861	835.764	547.316	356.379	1070.154	-46.582
1300	789.823	1354.386	873.276	625.442	357.481	1129.596	-45.387
1400	804.850	1413.482	909.771	705.195	358.927	1188.943	-44.359
1500	817.754	1469.462	945.235	786.341	360.641	1248.179	-43.465
1600	828.892	1522.603	979.674	868.687	362.509	1307.286	-42.678
1700	838.557	1573.151	1013.109	952.071	364.467	1366.252	-41.979
1800	846.982	1621.325	1045.572	1036.357	366.448	1425.158	-41.356
1900	854.362	1667.321	1077.094	1121.432	368.423	1483.908	-40.795
2000	860.855	1711.313	1107.713	1207.200	370.345	1542.578	-40.287
2100	866.591	1753.456	1137.466	1293.578	372.145	1601.142	-39.825
2200	871.678	1793.890	1166.391	1380.496	373.822	1659.626	-39.404
2300	876.208	1832.739	1194.524	1467.895	375.372	1718.036	-39.017
2400	880.257	1870.117	1221.900	1555.722	376.732	1776.339	-38.660
2500	883.888	1906.126	1248.553	1643.933	377.912	1834.690	-38.333
2600	887.155	1940.858	1274.516	1732.488	378.881	1892.894	-38.028
2700	890.103	1974.395	1299.820	1821.353	379.643	1951.128	-37.746
2800	892.773	2006.815	1324.494	1910.499	380.174	2009.358	-37.484
2900	895.196	2038.187	1348.566	1999.899	380.448	2067.526	-37.239
3000	897.403	2068.573	1372.063	2089.531	380.505	2125.712	-37.011
3100	899.416	2098.032	1395.008	2179.373	380.275	2183.833	-36.797
3200	901.259	2126.617	1417.427	2269.409	379.796	2242.030	-36.597
3300	902.949	2154.376	1439.340	2359.620	379.052	2300.281	-36.410
3400	904.502	2181.355	1460.769	2449.994	378.017	2358.482	-36.233
3500	905.932	2207.596	1481.734	2540.516	376.697	2416.701	-36.067
3600	907.253	2233.135	1502.253	2631.177	375.110	2475.039	-35.911
3700	908.474	2258.010	1522.344	2721.964	373.229	2533.441	-35.765
3800	909.605	2282.253	1542.024	2812.868	371.031	2591.844	-35.627
3900	910.656	2305.894	1561.309	2903.882	368.552	2650.263	-35.496
4000	911.632	2328.962	1580.213	2994.997	365.777	2708.872	-35.374
4100	912.541	2351.484	1598.751	3086.206	362.675	2767.489	-35.258
4200	913.390	2373.484	1616.936	3177.503	359.271	2826.178	-35.148
4300	914.182	2394.986	1634.781	3268.882	355.552	2884.871	-35.044
4400	914.923	2416.011	1652.298	3360.338	351.526	2943.737	-34.946
4500	915.617	2436.580	1669.499	3451.865	347.207	3002.746	-34.854
4600	916.269	2456.712	1686.394	3543.460	342.548	3061.862	-34.768
4700	916.881	2476.424	1702.994	3635.118	337.561	3120.983	-34.685
4800	917.456	2495.733	1719.309	3726.835	332.289	3180.306	-34.608
4900	917.998	2514.656	1735.348	3818.608	326.666	3239.623	-34.534
5000	918.508	2533.207	1751.121	3910.433	320.775	3299.223	-34.466

3.246. Benzo[*pqr*]picene



Other names: Naphtho[2,1-*a*]pyrene
Naphtho[3',4':3,4]pyrene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 189-96-8
Point Group: C_s

Length: 15.88 Å
Width: 9.198 Å
Breadth: 3.884 Å
L/B Ratio: 1.726

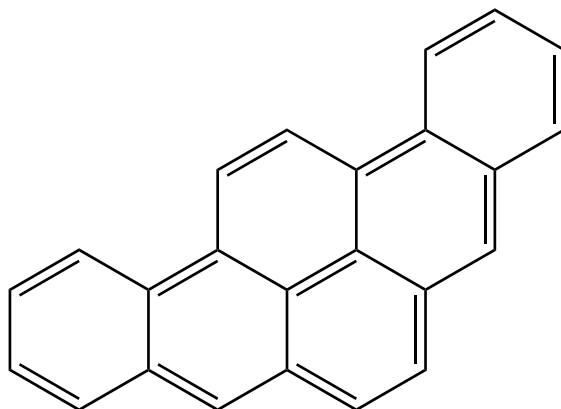
Cartesian coordinates:

C	5.1701	-0.7402	0.0000	C	-2.7706	2.5214	0.0000	H	5.5628	2.6332	0.0000
C	5.8030	0.4815	0.0000	C	-3.4520	1.2478	0.0000	H	3.0731	2.5351	0.0000
C	5.0485	1.6666	0.0000	C	-4.8426	1.1644	0.0000	H	1.2229	-3.1252	0.0000
C	3.6738	1.6128	0.0000	C	-5.4723	-0.0801	0.0000	H	3.7064	-2.9919	0.0000
C	3.7600	-0.8122	0.0000	C	-4.7300	-1.2494	0.0000	H	1.2836	2.4402	0.0000
C	3.0012	0.3712	0.0000	C	-2.6823	0.0591	0.0000	H	-0.9078	3.5594	0.0000
C	1.7415	-2.1542	0.0000	C	-3.3280	-1.1954	0.0000	H	-3.3841	3.4296	0.0000
C	3.0937	-2.0831	0.0000	C	-2.5268	-2.3874	0.0000	H	-5.4435	2.0808	0.0000
C	0.9313	-0.9688	0.0000	C	-1.1736	-2.3155	0.0000	H	-6.5664	-0.1301	0.0000
C	1.5555	0.2924	0.0000	C	-0.4886	-1.0521	0.0000	H	-5.2326	-2.2231	0.0000
C	0.7719	1.4641	0.0000	C	-1.2510	0.1270	0.0000	H	-3.0394	-3.3561	0.0000
C	-0.6091	1.3970	0.0000	H	5.7523	-1.6687	0.0000	H	-0.5565	-3.2271	0.0000
C	-1.4226	2.5916	0.0000	H	6.8964	0.5384	0.0000				

Table 3.246: Table of thermodynamic data as a function of temperature for Benzo[*pqr*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-44.230	369.372	369.372	∞
100	95.432	332.890	714.985	-38.210	393.223	432.727	-226.029
200	191.065	426.673	547.340	-24.133	380.617	477.253	-124.643
250	246.816	475.253	528.038	-13.196	374.678	502.099	-104.906
298.15	301.181	523.385	523.385	0.000	369.372	527.134	-92.350
300	303.246	525.254	523.391	0.559	369.176	528.111	-91.950
350	357.561	576.119	527.284	17.093	364.263	555.000	-82.828
400	407.994	627.207	536.582	36.250	359.973	582.540	-76.070
450	453.740	677.950	549.476	57.813	356.238	610.589	-70.874
500	494.679	727.917	564.830	81.544	352.982	639.047	-66.759
600	563.425	824.431	600.124	134.585	347.648	696.788	-60.659
700	617.872	915.531	638.742	193.752	343.698	755.314	-56.361
800	661.586	1000.993	678.740	257.802	340.973	814.306	-53.168
900	697.238	1081.044	719.042	325.802	339.314	873.570	-50.700
1000	726.706	1156.078	759.034	397.044	338.577	932.979	-48.733
1100	751.324	1226.529	798.364	470.982	338.585	992.432	-47.126
1200	772.065	1292.817	836.834	547.180	339.213	1051.841	-45.785
1300	789.666	1355.330	874.337	625.290	340.301	1111.188	-44.647
1400	804.695	1414.415	910.823	705.028	341.730	1170.441	-43.669
1500	817.603	1470.384	946.278	786.159	343.429	1229.584	-42.817
1600	828.746	1523.515	980.709	868.490	345.283	1288.599	-42.068
1700	838.417	1574.055	1014.138	951.859	347.226	1347.475	-41.402
1800	846.849	1622.221	1046.593	1036.132	349.193	1406.291	-40.809
1900	854.235	1668.210	1078.108	1121.194	351.155	1464.952	-40.274
2000	860.734	1712.196	1108.721	1206.949	353.064	1523.533	-39.790
2100	866.476	1754.333	1138.468	1293.316	354.853	1582.009	-39.350
2200	871.570	1794.761	1167.387	1380.223	356.519	1640.406	-38.947
2300	876.106	1833.606	1195.514	1467.611	358.058	1698.729	-38.579
2400	880.160	1870.980	1222.885	1555.428	359.408	1756.945	-38.238
2500	883.796	1906.985	1249.533	1643.629	360.579	1815.210	-37.926
2600	887.068	1941.713	1275.492	1732.175	361.539	1873.328	-37.635
2700	890.021	1975.247	1300.791	1821.032	362.292	1931.478	-37.366
2800	892.695	2007.664	1325.461	1910.170	362.815	1989.623	-37.116
2900	895.123	2039.033	1349.529	1999.563	363.082	2047.706	-36.882
3000	897.333	2069.417	1373.021	2089.187	363.132	2105.807	-36.665
3100	899.350	2098.874	1395.963	2179.023	362.895	2163.844	-36.460
3200	901.196	2127.457	1418.378	2269.052	362.410	2221.957	-36.269
3300	902.888	2155.214	1440.288	2359.257	361.659	2280.123	-36.091
3400	904.445	2182.192	1461.714	2449.625	360.619	2338.241	-35.922
3500	905.878	2208.430	1482.675	2540.142	359.293	2396.377	-35.763
3600	907.201	2233.968	1503.191	2630.797	357.701	2454.631	-35.615
3700	908.424	2258.842	1523.280	2721.579	355.815	2512.950	-35.476
3800	909.558	2283.083	1542.957	2812.479	353.612	2571.269	-35.344
3900	910.610	2306.723	1562.239	2903.488	351.128	2629.606	-35.219
4000	911.589	2329.790	1581.140	2994.598	348.348	2688.132	-35.103
4100	912.500	2352.311	1599.676	3085.803	345.242	2746.666	-34.992
4200	913.350	2374.310	1617.859	3177.096	341.834	2805.272	-34.888
4300	914.144	2395.811	1635.702	3268.471	338.112	2863.883	-34.789
4400	914.887	2416.836	1653.217	3359.923	334.082	2922.666	-34.696
4500	915.582	2437.404	1670.415	3451.447	329.759	2981.593	-34.609
4600	916.235	2457.534	1687.309	3543.038	325.096	3040.627	-34.527
4700	916.848	2477.246	1703.907	3634.693	320.107	3099.665	-34.448
4800	917.425	2496.554	1720.220	3726.407	314.832	3158.906	-34.375
4900	917.967	2515.477	1736.257	3818.176	309.206	3218.141	-34.305
5000	918.479	2534.027	1752.028	3909.999	303.311	3277.659	-34.241

3.247. Benzo[*rst*]pentaphene



Other names: Dibenzo[*a,i*]pyrene
 Dibenzo[*b,h*]pyrene
 3,4:9,10-Dibenzopyrene
 1,2:7,8-Dibenzopyrene
 4,5,8,9-Dibenzopyrene

Formula: C₂₄H₁₄
Mass: 302.368 g/mol
CAS Number: 189-55-9
Point Group: C_{2v}

Length: 15.90 Å
Width: 9.198 Å
Breadth: 3.884 Å
L/B Ratio: 1.729

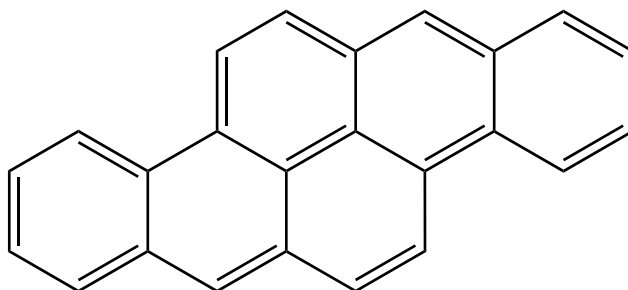
Cartesian coordinates:

C	4.9722	-1.8912	0.0000	C	-1.4146	-0.7271	0.0000	H	5.4760	1.4833	0.0000
C	5.6545	-0.6575	0.0000	C	-0.6831	-1.9489	0.0000	H	3.0525	-2.8770	0.0000
C	4.9520	0.5207	0.0000	C	0.6800	-1.9500	0.0000	H	3.3565	2.6794	0.0000
C	3.6008	-1.9225	0.0000	C	1.4135	-0.7293	0.0000	H	1.2409	3.9049	0.0000
C	2.8508	-0.7208	0.0000	C	0.7144	0.4839	0.0000	H	-1.2349	3.9068	0.0000
C	3.5341	0.5107	0.0000	C	-2.8519	-0.7164	0.0000	H	-3.3523	2.6846	0.0000
C	2.8016	1.7330	0.0000	C	-3.5334	0.5162	0.0000	H	-1.2540	-2.8903	0.0000
C	1.4312	1.7282	0.0000	C	-4.9512	0.5283	0.0000	H	1.2495	-2.8922	0.0000
C	0.6749	2.9660	0.0000	C	-5.6555	-0.6488	0.0000	H	-5.4738	1.4917	0.0000
C	-0.6703	2.9670	0.0000	C	-4.9751	-1.8835	0.0000	H	-6.7504	-0.6407	0.0000
C	-1.4285	1.7304	0.0000	C	-3.6037	-1.9169	0.0000	H	-5.5521	-2.8139	0.0000
C	-2.7989	1.7373	0.0000	H	5.5479	-2.8225	0.0000	H	-3.0568	-2.8722	0.0000
C	-0.7136	0.4851	0.0000	H	6.7494	-0.6510	0.0000				

Table 3.247: Table of thermodynamic data as a function of temperature for Benzo[*rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-44.371	375.910	375.910	∞
100	95.937	326.222	709.774	-38.355	399.615	439.786	-229.716
200	191.828	420.489	541.529	-24.208	387.080	484.953	-126.654
250	247.570	469.238	522.169	-13.233	381.179	510.104	-106.578
298.15	301.956	517.504	517.504	0.000	375.910	535.425	-93.802
300	304.021	519.378	517.510	0.561	375.715	536.413	-93.396
350	358.361	570.365	521.412	17.133	370.841	563.593	-84.110
400	408.806	621.560	530.732	36.331	366.592	591.418	-77.230
450	454.545	672.399	543.654	57.935	362.897	619.747	-71.937
500	495.462	722.449	559.039	81.705	359.681	648.480	-67.745
600	564.141	819.101	594.399	134.821	354.422	706.760	-61.528
700	618.512	910.305	633.081	194.057	350.540	765.814	-57.145
800	662.155	995.848	673.139	258.167	347.875	825.325	-53.887
900	697.744	1075.962	713.495	326.220	346.270	885.099	-51.369
1000	727.158	1151.047	753.536	397.511	345.581	945.014	-49.361
1100	751.729	1221.539	792.911	471.491	345.632	1004.969	-47.721
1200	772.430	1287.860	831.421	547.728	346.299	1064.875	-46.352
1300	789.995	1350.400	868.960	625.872	347.420	1124.716	-45.191
1400	804.993	1409.508	905.479	705.641	348.881	1184.461	-44.192
1500	817.873	1465.497	940.964	786.800	350.608	1244.093	-43.322
1600	828.993	1518.645	975.422	869.157	352.488	1303.597	-42.557
1700	838.642	1569.199	1008.875	952.550	354.455	1362.958	-41.878
1800	847.055	1617.378	1041.353	1036.844	356.443	1422.259	-41.272
1900	854.425	1663.377	1072.890	1121.926	358.425	1481.404	-40.726
2000	860.909	1707.372	1103.522	1207.700	360.353	1540.468	-40.232
2100	866.637	1749.517	1133.288	1294.083	362.158	1599.426	-39.783
2200	871.719	1789.953	1162.223	1381.006	363.840	1658.304	-39.372
2300	876.245	1828.804	1190.366	1468.408	365.393	1717.107	-38.996
2400	880.289	1866.184	1217.751	1556.238	366.756	1775.804	-38.649
2500	883.916	1902.194	1244.413	1644.452	367.940	1834.548	-38.330
2600	887.180	1936.926	1270.384	1733.010	368.912	1893.145	-38.033
2700	890.126	1970.465	1295.696	1821.877	369.675	1951.773	-37.759
2800	892.793	2002.886	1320.377	1911.026	370.209	2010.396	-37.504
2900	895.215	2034.258	1344.455	2000.428	370.485	2068.957	-37.265
3000	897.420	2064.645	1367.958	2090.061	370.543	2127.535	-37.043
3100	899.432	2094.105	1390.909	2179.905	370.315	2186.049	-36.834
3200	901.273	2122.690	1413.333	2269.942	369.838	2244.639	-36.639
3300	902.962	2150.450	1435.251	2360.155	369.095	2303.282	-36.457
3400	904.514	2177.429	1456.685	2450.530	368.062	2361.876	-36.285
3500	905.943	2203.670	1477.654	2541.054	366.743	2420.488	-36.123
3600	907.263	2229.210	1498.178	2631.715	365.157	2479.218	-35.972
3700	908.484	2254.085	1518.273	2722.503	363.277	2538.013	-35.830
3800	909.614	2278.327	1537.957	2813.409	361.079	2596.808	-35.695
3900	910.664	2301.969	1557.245	2904.423	358.601	2655.620	-35.567
4000	911.640	2325.037	1576.153	2995.539	355.827	2714.622	-35.449
4100	912.549	2347.559	1594.694	3086.749	352.726	2773.631	-35.336
4200	913.396	2369.560	1612.882	3178.047	349.322	2832.712	-35.229
4300	914.188	2391.062	1630.730	3269.426	345.604	2891.798	-35.128
4400	914.929	2412.087	1648.250	3360.883	341.579	2951.056	-35.033
4500	915.623	2432.656	1665.454	3452.411	337.260	3010.458	-34.944
4600	916.274	2452.788	1682.352	3544.006	332.602	3069.966	-34.860
4700	916.886	2472.500	1698.954	3635.664	327.616	3129.479	-34.780
4800	917.461	2491.810	1715.272	3727.382	322.345	3189.194	-34.705
4900	918.002	2510.733	1731.313	3819.155	316.722	3248.903	-34.633
5000	918.512	2529.284	1747.088	3910.981	310.831	3308.896	-34.567

3.248. Dibenzo[*b,def*]chrysene



Other names: Dibenzo[*a,h*]pyrene
3,4:8,9-Dibenzpyrene

Formula: C₂₄H₁₄

Mass: 302.368 g/mol

CAS Number: 189-64-0

Point Group: C_{2h}

Length: 15.88 Å

Width: 9.202 Å

Breadth: 3.890 Å

L/B Ratio: 1.726

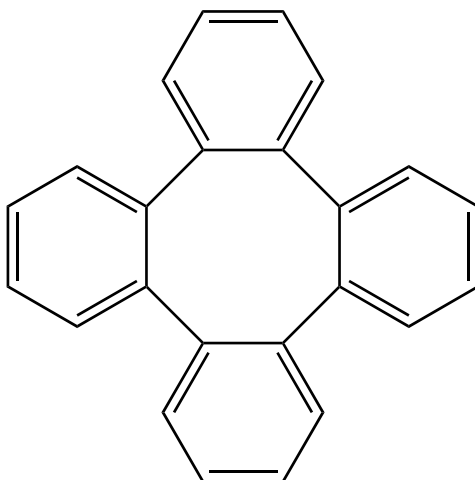
Cartesian coordinates:

C	5.4064	-1.0576	0.0000	C	0.6966	0.1762	0.0000	H	5.0534	2.3393	0.0000
C	5.7598	0.3142	0.0000	C	-0.6966	-0.1761	0.0000	H	3.8016	-2.4933	0.0000
C	4.7895	1.2755	0.0000	C	-1.0705	-1.5533	0.0000	H	2.6992	2.9627	0.0000
C	4.0926	-1.4317	0.0000	C	-0.0315	-2.5534	0.0000	H	0.3325	3.6075	0.0000
C	3.0561	-0.4553	0.0000	C	1.2733	-2.2027	0.0000	H	-2.0706	2.9620	0.0000
C	3.4111	0.9127	0.0000	C	-3.4110	-0.9127	0.0000	H	-2.6990	-2.9627	0.0000
C	2.4068	1.9053	0.0000	C	-3.0561	0.4553	0.0000	H	-0.3324	-3.6074	0.0000
C	1.0705	1.5533	0.0000	C	-4.0927	1.4317	0.0000	H	2.0706	-2.9620	0.0000
C	0.0315	2.5535	0.0000	C	-5.4065	1.0575	0.0000	H	-3.8016	2.4932	0.0000
C	-1.2733	2.2027	0.0000	C	-5.7598	-0.3143	0.0000	H	-6.2005	1.8114	0.0000
C	-1.6796	0.8208	0.0000	C	-4.7895	-1.2756	0.0000	H	-6.8193	-0.5903	0.0000
C	-2.4067	-1.9053	0.0000	H	6.2003	-1.8116	0.0000	H	-5.0533	-2.3394	0.0000
C	1.6795	-0.8208	0.0000	H	6.8193	0.5902	0.0000				

Table 3.248: Table of thermodynamic data as a function of temperature for Dibenzo[*b,def*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-44.295	385.553	385.553	∞
100	95.617	326.141	709.089	-38.295	409.318	449.498	-234.789
200	191.538	420.185	541.082	-24.179	396.751	494.685	-129.196
250	247.288	468.871	521.745	-13.219	390.836	519.853	-108.615
298.15	301.638	517.085	517.085	0.000	385.553	545.193	-95.514
300	303.701	518.957	517.090	0.560	385.358	546.182	-95.097
350	357.986	569.890	520.989	17.115	380.466	573.384	-85.571
400	408.381	621.032	530.299	36.293	376.197	601.234	-78.511
450	454.087	671.818	543.207	57.875	372.480	629.591	-73.079
500	494.986	721.819	558.576	81.621	369.240	658.354	-68.776
600	563.664	818.384	593.901	134.690	363.933	716.702	-62.393
700	618.059	909.516	632.547	193.879	360.005	775.831	-57.892
800	661.734	995.000	672.569	257.945	357.296	835.424	-54.546
900	697.357	1075.067	712.891	325.958	355.651	895.286	-51.960
1000	726.803	1150.112	752.901	397.211	354.924	955.292	-49.898
1100	751.404	1220.572	792.247	471.157	354.941	1015.342	-48.214
1200	772.132	1286.866	830.731	547.363	355.577	1075.346	-46.808
1300	789.723	1349.384	868.246	625.479	356.670	1135.288	-45.615
1400	804.744	1408.472	904.742	705.222	358.105	1195.135	-44.590
1500	817.645	1464.445	940.207	786.358	359.809	1254.872	-43.698
1600	828.783	1517.579	974.646	868.692	361.666	1314.481	-42.913
1700	838.449	1568.120	1008.082	952.065	363.613	1373.950	-42.215
1800	846.878	1616.289	1040.544	1036.341	365.583	1433.360	-41.594
1900	854.261	1662.279	1072.065	1121.406	367.548	1492.614	-41.034
2000	860.757	1706.266	1102.684	1207.164	369.460	1551.788	-40.528
2100	866.497	1748.404	1132.436	1293.532	371.250	1610.857	-40.067
2200	871.589	1788.833	1161.360	1380.441	372.918	1669.847	-39.646
2300	876.123	1827.679	1189.491	1467.831	374.459	1728.762	-39.261
2400	880.176	1865.053	1216.866	1555.650	375.811	1787.572	-38.905
2500	883.811	1901.059	1243.518	1643.853	376.984	1846.429	-38.578
2600	887.081	1935.787	1269.480	1732.400	377.945	1905.139	-38.274
2700	890.033	1969.323	1294.782	1821.258	378.699	1963.881	-37.993
2800	892.706	2001.740	1319.455	1910.397	379.223	2022.619	-37.732
2900	895.133	2033.109	1343.526	1999.791	379.491	2081.294	-37.487
3000	897.342	2063.494	1367.021	2089.417	379.542	2139.988	-37.260
3100	899.359	2092.951	1389.966	2179.253	379.306	2198.617	-37.046
3200	901.204	2121.534	1412.383	2269.283	378.822	2257.322	-36.846
3300	902.897	2149.291	1434.295	2359.489	378.072	2316.081	-36.660
3400	904.452	2176.269	1455.723	2449.858	377.033	2374.791	-36.483
3500	905.885	2202.508	1476.686	2540.376	375.707	2433.519	-36.318
3600	907.208	2228.046	1497.204	2631.031	374.116	2492.366	-36.163
3700	908.431	2252.920	1517.294	2721.814	372.231	2551.277	-36.017
3800	909.564	2277.161	1536.973	2812.714	370.028	2610.188	-35.879
3900	910.616	2300.801	1556.257	2903.724	367.545	2669.117	-35.748
4000	911.594	2323.869	1575.160	2994.835	364.766	2728.236	-35.626
4100	912.505	2346.390	1593.697	3086.040	361.660	2787.362	-35.511
4200	913.355	2368.389	1611.881	3177.334	358.253	2846.560	-35.401
4300	914.148	2389.890	1629.725	3268.710	354.530	2905.763	-35.297
4400	914.891	2410.914	1647.241	3360.162	350.502	2965.138	-35.200
4500	915.587	2431.483	1664.441	3451.686	346.179	3024.657	-35.109
4600	916.239	2451.613	1681.336	3543.278	341.517	3084.283	-35.022
4700	916.852	2471.325	1697.935	3634.933	336.528	3143.913	-34.940
4800	917.428	2490.634	1714.249	3726.647	331.253	3203.747	-34.863
4900	917.971	2509.556	1730.287	3818.417	325.627	3263.573	-34.789
5000	918.482	2528.107	1746.059	3910.240	319.733	3323.684	-34.722

3.249. Tetraphenylene



Other names: Tetrabenzocyclooctatetraene

Formula: $C_{24}H_{16}$

Mass: 304.39 g/mol

CAS Number: 212-74-8

Point Group: D_{2d}

Length: 9.781 Å

Width: 9.738 Å

Breadth: 8.837 Å

L/B Ratio: 1.004

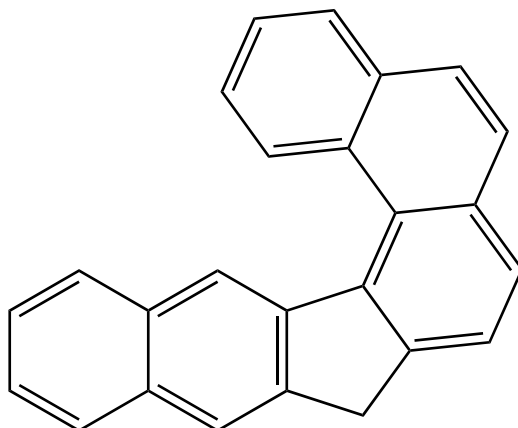
Cartesian coordinates:

C	0.0067	1.3759	0.0242	C	0.4493	3.3465	-4.7307	H	2.2216	3.6377	1.9496
C	0.0297	-0.0284	0.0893	C	-0.7606	2.6482	-4.7209	H	2.4379	6.1135	2.0060
C	1.2327	-0.7353	0.1300	C	-1.4538	2.4861	-3.5200	H	1.6277	7.4711	0.0636
C	2.4432	-0.0383	0.1182	C	-0.9549	3.0012	-2.3109	H	0.6195	6.3272	-1.8995
C	2.4352	1.3568	0.0657	C	-1.7676	2.8393	-1.0667	H	1.8944	4.4240	-3.5407
C	1.2316	2.0810	0.0121	C	-1.3145	2.0756	0.0329	H	1.0035	3.4803	-5.6628
C	1.2886	3.5751	0.0075	C	-2.1585	1.9177	1.1462	H	-1.1654	2.2289	-5.6452
C	1.8690	4.2346	1.1050	C	-3.4238	2.5058	1.1897	H	-2.4014	1.9421	-3.5085
C	1.9917	5.6248	1.1365	C	-3.8720	3.2597	0.1025	H	-1.8049	1.3249	1.9933
C	1.5398	6.3820	0.0531	C	-3.0486	3.4161	-1.0139	H	-4.0563	2.3756	2.0712
C	0.9721	5.7393	-1.0486	H	-0.9198	-0.5690	0.1000	H	-4.8599	3.7263	0.1215
C	0.8327	4.3410	-1.0894	H	1.2229	-1.8273	0.1700	H	-3.3950	4.0031	-1.8680
C	0.2690	3.7079	-2.3209	H	3.3932	-0.5775	0.1487				
C	0.9504	3.8740	-3.5394	H	3.3794	1.9067	0.0576				

Table 3.249: Table of thermodynamic data as a function of temperature for Tetraphenylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-48.130	448.333	448.333	∞
100	111.153	334.726	746.622	-41.190	474.671	524.065	-273.738
200	205.356	439.010	567.054	-25.609	460.876	578.927	-151.197
250	261.701	490.818	546.609	-13.948	454.265	609.205	-127.284
298.15	317.627	541.695	541.695	0.000	448.333	639.598	-112.053
300	319.763	543.666	541.701	0.590	448.114	640.783	-111.568
350	376.133	597.230	545.802	18.000	442.628	673.341	-100.489
400	428.637	650.933	555.589	38.138	437.863	706.625	-92.274
450	476.284	704.220	569.149	60.782	433.747	740.472	-85.950
500	518.909	756.651	585.286	85.682	430.199	774.766	-80.938
600	590.472	857.842	622.355	141.292	424.505	844.245	-73.497
700	647.225	953.289	662.884	203.284	420.440	914.550	-68.243
800	692.934	1042.804	704.841	270.370	417.799	985.323	-64.334
900	730.369	1126.651	747.101	341.595	416.392	1056.347	-61.308
1000	761.445	1205.261	789.028	416.233	416.046	1127.481	-58.892
1100	787.512	1279.092	830.258	493.718	416.563	1198.614	-56.916
1200	809.555	1348.586	870.585	573.601	417.798	1269.652	-55.265
1300	828.319	1414.146	909.900	655.520	419.573	1340.574	-53.864
1400	844.385	1476.134	948.152	739.175	421.756	1411.346	-52.657
1500	858.214	1534.874	985.326	824.322	424.263	1481.953	-51.605
1600	870.177	1590.653	1021.430	910.756	426.969	1552.376	-50.679
1700	880.575	1643.726	1056.487	998.306	429.799	1622.603	-49.856
1800	889.654	1694.321	1090.528	1086.827	432.680	1692.721	-49.120
1900	897.617	1742.640	1123.588	1176.199	435.580	1762.631	-48.457
2000	904.631	1788.864	1155.705	1266.319	438.444	1832.412	-47.857
2100	910.833	1833.154	1186.917	1357.099	441.199	1902.039	-47.310
2200	916.340	1875.656	1217.264	1448.463	443.843	1971.541	-46.809
2300	921.247	1916.499	1246.783	1540.347	446.367	2040.923	-46.350
2400	925.635	1955.801	1275.512	1632.695	448.708	2110.157	-45.925
2500	929.573	1993.669	1303.486	1725.459	450.872	2179.399	-45.535
2600	933.118	2030.198	1330.738	1818.596	452.825	2248.453	-45.171
2700	936.319	2065.475	1357.301	1912.071	454.572	2317.499	-44.834
2800	939.219	2099.580	1383.205	2005.850	456.087	2386.508	-44.520
2900	941.852	2132.585	1408.480	2099.906	457.343	2455.416	-44.226
3000	944.250	2164.556	1433.152	2194.213	458.378	2524.308	-43.951
3100	946.440	2195.554	1457.248	2288.749	459.122	2593.105	-43.693
3200	948.444	2225.635	1480.793	2383.494	459.611	2661.945	-43.451
3300	950.282	2254.848	1503.808	2478.432	459.829	2730.808	-43.224
3400	951.972	2283.243	1526.317	2573.546	459.751	2799.594	-43.010
3500	953.529	2310.861	1548.340	2668.822	459.379	2868.370	-42.807
3600	954.967	2337.743	1569.896	2764.248	458.733	2937.236	-42.617
3700	956.297	2363.926	1591.004	2859.812	457.785	3006.143	-42.438
3800	957.529	2389.446	1611.682	2955.504	456.509	3075.021	-42.268
3900	958.673	2414.333	1631.945	3051.315	454.944	3143.896	-42.107
4000	959.736	2438.618	1651.809	3147.236	453.073	3212.936	-41.956
4100	960.727	2462.329	1671.290	3243.259	450.864	3281.960	-41.812
4200	961.651	2485.491	1690.401	3339.379	448.344	3351.034	-41.675
4300	962.515	2508.130	1709.156	3435.588	445.497	3420.092	-41.545
4400	963.323	2530.267	1727.567	3531.880	442.333	3489.304	-41.422
4500	964.080	2551.924	1745.646	3628.251	438.863	3558.642	-41.307
4600	964.790	2573.121	1763.405	3724.694	435.043	3628.064	-41.197
4700	965.457	2593.877	1780.855	3821.207	430.884	3697.472	-41.092
4800	966.084	2614.210	1798.005	3917.784	426.429	3767.066	-40.993
4900	966.674	2634.136	1814.866	4014.423	421.611	3836.636	-40.898
5000	967.231	2653.671	1831.448	4111.118	416.515	3906.479	-40.810

3.250. 9H-Benz[5,6]indeno[2,1-c]phenanthrene



Formula: C₂₅H₁₆
Mass: 316.395 g/mol
CAS Number: 192-84-7
Point Group: C₁

Length: 13.97 Å
Width: 11.11 Å
Breadth: 5.574 Å
L/B Ratio: 1.257

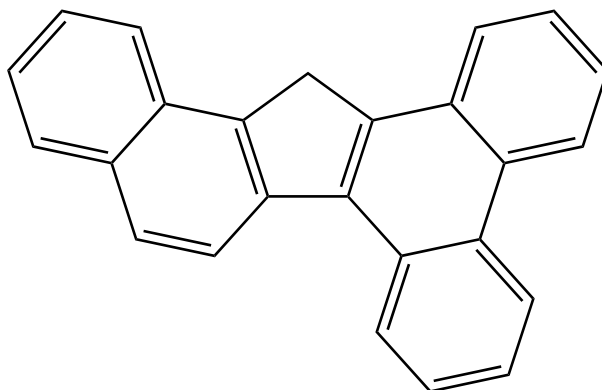
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C	-5.0124	-0.1892	0.0532	C	2.9320	-1.3765	-0.3029	H	-0.7060	1.3566	-0.5921
C	-3.3319	1.9433	-0.6251	C	4.1722	-0.7830	-0.7278	H	-0.9940	-3.4937	1.5079
C	-2.7582	0.6872	-0.2923	C	4.3205	0.5598	-0.7745	H	-1.1979	-3.8419	-0.2223
C	-3.6072	-0.3891	0.0424	C	2.0734	0.8665	0.1871	H	1.5702	-4.4739	0.2250
C	-3.0470	-1.6663	0.3375	C	3.2884	1.4189	-0.2626	H	3.7278	-3.3880	-0.4210
C	-1.3432	0.5149	-0.2912	C	3.5277	2.8023	-0.1295	H	4.9841	-1.4511	-1.0382
C	-0.8158	-0.6947	0.0665	C	2.6139	3.6070	0.5134	H	5.2413	1.0181	-1.1528
C	-1.6925	-1.8059	0.3306	C	1.4571	3.0413	1.0690	H	4.4570	3.2250	-0.5283
C	-0.8890	-3.0600	0.4958	C	1.1961	1.6970	0.9146	H	2.7956	4.6817	0.6158
C	0.5691	-1.1874	0.1171	H	-5.1351	3.0777	-0.8650	H	0.7642	3.6736	1.6339
C	0.5133	-2.5861	0.2493	H	-6.6231	1.1919	-0.2564	H	0.3109	1.2547	1.3905
C	1.6438	-3.3881	0.1103	H	-5.6644	-1.0290	0.3187				

Table 3.250: Table of thermodynamic data as a function of temperature for 9*H*-Benz[5,6]indeno[2,1-*c*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.044	421.290	421.290	∞
100	105.944	344.619	759.211	-41.459	448.350	496.849	-259.522
200	207.204	447.442	577.680	-26.048	434.059	551.040	-143.914
250	266.312	499.972	556.860	-14.222	427.317	581.066	-121.405
298.15	324.336	551.847	551.847	0.000	421.290	611.239	-107.084
300	326.544	553.860	551.854	0.602	421.068	612.417	-106.629
350	384.739	608.610	556.044	18.398	415.497	644.761	-96.223
400	438.862	663.570	566.051	39.007	410.650	677.844	-88.515
450	487.984	718.147	579.925	62.200	406.455	711.499	-82.587
500	531.956	771.882	596.442	87.720	402.829	745.611	-77.892
600	605.849	875.665	634.406	144.755	396.982	814.748	-70.929
700	664.481	973.629	675.941	208.381	392.779	884.735	-66.018
800	711.678	1065.549	718.959	277.271	390.020	955.208	-62.367
900	750.277	1151.674	762.306	350.431	388.513	1025.946	-59.543
1000	782.264	1232.430	805.323	427.107	388.082	1096.804	-57.290
1100	809.044	1308.281	847.634	506.711	388.524	1167.671	-55.447
1200	831.648	1379.673	889.026	588.777	389.691	1238.447	-53.907
1300	850.857	1447.019	929.383	672.927	391.398	1309.113	-52.600
1400	867.279	1510.691	968.652	758.855	393.514	1379.636	-51.474
1500	881.395	1571.021	1006.816	846.306	395.951	1449.997	-50.492
1600	893.592	1628.303	1043.884	935.070	398.582	1520.180	-49.628
1700	904.182	1682.802	1079.878	1024.971	401.331	1590.171	-48.859
1800	913.421	1734.751	1114.828	1115.862	404.125	1660.060	-48.173
1900	921.518	1784.359	1148.771	1207.618	406.929	1729.743	-47.553
2000	928.644	1831.812	1181.745	1300.133	409.690	1799.304	-46.992
2100	934.942	1877.276	1213.791	1393.319	412.333	1868.716	-46.481
2200	940.531	1920.901	1244.947	1487.098	414.855	1938.009	-46.013
2300	945.508	1962.821	1275.254	1581.405	417.248	2007.187	-45.584
2400	949.958	2003.157	1304.748	1676.182	419.448	2076.222	-45.187
2500	953.949	2042.019	1333.467	1771.381	421.462	2145.274	-44.822
2600	957.541	2079.505	1361.444	1866.958	423.255	2214.141	-44.482
2700	960.783	2115.704	1388.713	1962.877	424.832	2283.009	-44.167
2800	963.719	2150.700	1415.305	2059.105	426.168	2351.846	-43.873
2900	966.385	2184.565	1441.251	2155.612	427.233	2420.588	-43.599
3000	968.813	2217.369	1466.577	2252.374	428.069	2489.322	-43.342
3100	971.028	2249.173	1491.312	2349.368	428.603	2557.963	-43.100
3200	973.056	2280.034	1515.480	2446.573	428.872	2626.658	-42.875
3300	974.915	2310.005	1539.104	2543.973	428.860	2695.385	-42.663
3400	976.624	2339.135	1562.208	2641.551	428.541	2764.038	-42.463
3500	978.199	2367.468	1584.813	2739.294	427.919	2832.687	-42.275
3600	979.653	2395.046	1606.938	2837.187	427.012	2901.438	-42.098
3700	980.997	2421.906	1628.603	2935.221	425.793	2970.237	-41.931
3800	982.243	2448.084	1649.825	3033.383	424.236	3039.013	-41.773
3900	983.399	2473.613	1670.622	3131.666	422.380	3107.791	-41.623
4000	984.474	2498.524	1691.009	3230.060	420.208	3176.747	-41.483
4100	985.475	2522.846	1711.003	3328.558	417.688	3245.692	-41.350
4200	986.409	2546.605	1730.616	3427.153	414.846	3314.694	-41.223
4300	987.281	2569.826	1749.864	3525.838	411.667	3383.685	-41.103
4400	988.097	2592.533	1768.758	3624.607	408.161	3452.840	-40.990
4500	988.862	2614.747	1787.312	3723.456	404.341	3522.132	-40.883
4600	989.579	2636.489	1805.537	3822.378	400.158	3591.516	-40.782
4700	990.253	2657.778	1823.444	3921.370	395.626	3660.890	-40.685
4800	990.887	2678.633	1841.044	4020.428	390.789	3730.462	-40.595
4900	991.483	2699.070	1858.347	4119.546	385.578	3800.013	-40.508
5000	992.045	2719.107	1875.362	4218.723	380.080	3869.851	-40.427

3.251. 1*H*-Benz[4,5]indeno[1,2-*l*]phenanthrene



Formula: C₂₅H₁₆
Mass: 316.395 g/mol
CAS Number: 873972-33-9
Point Group: C_s

Length: 15.10 Å
Width: 11.22 Å
Breadth: 4.178 Å
L/B Ratio: 1.346

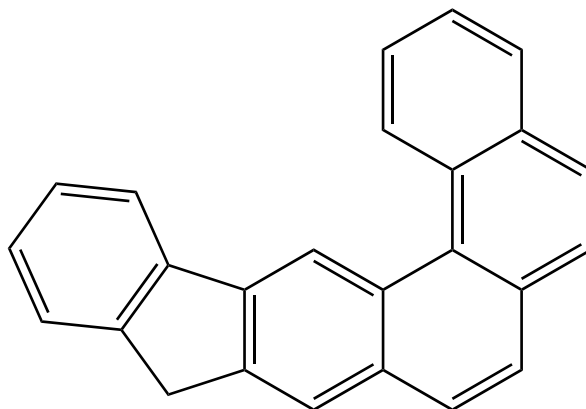
Cartesian coordinates:

C	5.9612	0.1593	0.0000	C	-2.8969	-0.9694	0.0000	H	6.0494	-2.0081	0.0000
C	5.1637	1.2710	0.0000	C	-4.1059	-1.7001	0.0000	H	3.3737	3.2776	0.0000
C	4.0301	-1.2914	0.0000	C	-4.0996	-3.0757	0.0000	H	0.9064	3.0632	0.0000
C	5.3888	-1.1350	0.0000	C	-2.8829	-3.7783	0.0000	H	1.1202	-2.1213	0.8895
C	3.1787	-0.1533	0.0000	C	-1.6911	-3.0920	0.0000	H	1.1202	-2.1213	-0.8895
C	3.7478	1.1406	0.0000	C	-2.8894	0.4793	0.0000	H	-5.0567	-1.1456	0.0000
C	2.9065	2.2859	0.0000	C	-1.6718	1.1957	0.0000	H	-5.0428	-3.6317	0.0000
C	1.5403	2.1675	0.0000	C	-1.7114	2.6063	0.0000	H	-2.8918	-4.8731	0.0000
C	1.7700	-0.2513	-0.0000	C	-2.9097	3.2824	0.0000	H	-0.7363	-3.6305	-0.0000
C	0.9573	0.8839	0.0000	C	-4.1195	2.5718	0.0000	H	-0.7717	3.1736	0.0000
C	0.9281	-1.4917	-0.0000	C	-4.1062	1.1968	0.0000	H	-2.9262	4.3772	0.0000
C	-0.4661	-0.9329	-0.0000	H	7.0518	0.2573	0.0000	H	-5.0689	3.1169	0.0000
C	-0.4459	0.4493	0.0000	H	5.6019	2.2755	0.0000	H	-5.0505	0.6310	0.0000
C	-1.6812	-1.6801	0.0000	H	3.5749	-2.2884	-0.0000				

Table 3.251: Table of thermodynamic data as a function of temperature for 1*H*-Benz[4,5]indeno[1,2-*l*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.812	402.805	402.805	∞
100	109.866	356.501	775.108	-41.861	429.463	476.774	-249.036
200	209.092	461.441	592.219	-26.156	415.466	529.647	-138.327
250	267.360	514.298	571.329	-14.258	408.796	558.964	-116.787
298.15	324.809	566.305	566.305	0.000	402.805	588.443	-103.091
300	327.000	568.321	566.311	0.603	402.584	589.594	-102.655
350	384.809	623.109	570.506	18.411	397.025	621.214	-92.709
400	438.694	678.062	580.517	39.018	392.175	653.572	-85.346
450	487.673	732.611	594.392	62.198	387.968	686.504	-79.686
500	531.562	786.307	610.907	87.700	384.324	719.893	-75.205
600	605.376	890.010	648.858	144.691	378.433	787.591	-68.565
700	663.979	987.899	690.373	208.269	374.181	856.148	-63.885
800	711.165	1079.751	733.366	277.108	371.371	925.198	-60.408
900	749.764	1165.816	776.687	350.216	369.813	994.518	-57.719
1000	781.758	1246.519	819.677	426.841	369.331	1063.965	-55.575
1100	808.552	1322.321	861.962	506.395	369.723	1133.425	-53.821
1200	831.175	1393.672	903.328	588.413	370.841	1202.799	-52.355
1300	850.406	1460.981	943.660	672.517	372.503	1272.068	-51.111
1400	866.851	1524.620	982.905	758.401	374.575	1341.196	-50.040
1500	880.991	1584.921	1021.047	845.811	376.970	1410.166	-49.105
1600	893.211	1642.178	1058.094	934.535	379.562	1478.960	-48.282
1700	903.825	1696.655	1094.067	1024.399	382.274	1547.565	-47.550
1800	913.086	1748.584	1128.998	1115.255	385.033	1616.069	-46.896
1900	921.204	1798.174	1162.923	1206.979	387.805	1684.370	-46.306
2000	928.350	1845.611	1195.880	1299.464	390.535	1752.550	-45.771
2100	934.666	1891.062	1227.909	1392.621	393.149	1820.583	-45.284
2200	940.272	1934.674	1259.050	1486.373	395.645	1888.498	-44.838
2300	945.265	1976.583	1289.342	1580.655	398.013	1956.299	-44.428
2400	949.729	2016.910	1318.823	1675.409	400.189	2023.958	-44.049
2500	953.734	2055.762	1347.528	1770.585	402.181	2091.636	-43.701
2600	957.339	2093.240	1375.493	1866.142	403.954	2159.129	-43.377
2700	960.593	2129.432	1402.750	1962.041	405.511	2226.623	-43.076
2800	963.540	2164.421	1429.331	2058.250	406.828	2294.088	-42.796
2900	966.215	2198.280	1455.266	2154.740	407.876	2361.458	-42.534
3000	968.652	2231.078	1480.583	2251.486	408.695	2428.821	-42.289
3100	970.876	2262.877	1505.308	2348.464	409.213	2496.091	-42.058
3200	972.911	2293.733	1529.466	2445.654	409.468	2563.416	-41.843
3300	974.778	2323.700	1553.082	2543.040	409.442	2630.773	-41.641
3400	976.494	2352.826	1576.178	2640.605	409.110	2698.057	-41.450
3500	978.076	2381.155	1598.774	2738.335	408.474	2765.338	-41.270
3600	979.535	2408.729	1620.892	2836.216	407.556	2832.720	-41.101
3700	980.885	2435.586	1642.549	2934.238	406.326	2900.150	-40.942
3800	982.136	2461.762	1663.764	3032.390	404.757	2967.559	-40.791
3900	983.297	2487.288	1684.554	3130.662	402.891	3034.969	-40.648
4000	984.376	2512.197	1704.935	3229.046	400.709	3102.557	-40.514
4100	985.382	2536.516	1724.922	3327.535	398.180	3170.135	-40.387
4200	986.320	2560.273	1744.530	3426.121	395.328	3237.771	-40.267
4300	987.196	2583.492	1763.772	3524.797	392.140	3305.395	-40.152
4400	988.015	2606.197	1782.661	3623.558	388.626	3373.184	-40.044
4500	988.783	2628.409	1801.209	3722.398	384.798	3441.109	-39.943
4600	989.504	2650.149	1819.429	3821.313	380.608	3509.127	-39.847
4700	990.180	2671.437	1837.331	3920.297	376.068	3577.135	-39.755
4800	990.817	2692.290	1854.926	4019.348	371.224	3645.341	-39.669
4900	991.416	2712.726	1872.225	4118.460	366.006	3713.527	-39.586
5000	991.981	2732.762	1889.236	4217.630	360.501	3781.999	-39.509

3.252. 1*H*-Benz[*g*]indeno[2,1-*a*]phenanthrene



Formula: C₂₅H₁₆
Mass: 316.395 g/mol
Point Group: C₁

Length: 14.47 Å
Width: 10.66 Å
Breadth: 5.043 Å
L/B Ratio: 1.357

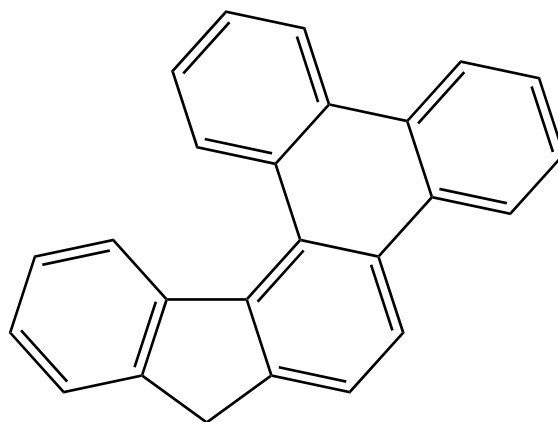
Cartesian coordinates:

C	-4.4991	-2.4550	0.4431	C	2.3406	2.9972	0.0668	H	-2.3309	-2.5833	0.5306
C	-5.6050	-1.6333	0.2597	C	1.9013	0.5752	0.0011	H	-4.0833	2.0414	-1.2737
C	-5.4532	-0.2657	0.0135	C	2.7858	1.6454	0.1843	H	-4.1455	2.3617	0.4733
C	-3.2030	-1.9376	0.3855	C	4.1638	1.4209	0.4964	H	-1.5873	3.6106	-0.4781
C	-3.0484	-0.5839	0.1413	C	4.6576	0.1610	0.5720	H	-0.2500	-1.1585	0.3214
C	-4.1740	0.2539	-0.0439	C	2.4738	-0.7510	-0.1180	H	0.6930	4.3057	-0.3188
C	-3.7402	1.6720	-0.2898	C	3.8287	-0.9510	0.2244	H	3.0785	3.8029	0.1577
C	-1.8409	0.2310	0.0227	C	4.4005	-2.2444	0.1708	H	4.8038	2.2889	0.6937
C	-2.2419	1.5808	-0.2209	C	3.6676	-3.3125	-0.2821	H	5.6988	-0.0249	0.8589
C	-1.3019	2.5644	-0.3222	C	2.3472	-3.1093	-0.7190	H	5.4423	-2.3777	0.4848
C	-0.5200	-0.1153	0.1085	C	1.7711	-1.8646	-0.6405	H	4.1054	-4.3149	-0.3239
C	0.4864	0.8757	-0.0555	H	-4.6433	-3.5232	0.6358	H	1.7818	-3.9524	-1.1297
C	0.0729	2.2193	-0.2038	H	-6.6118	-2.0611	0.3086	H	0.7453	-1.7343	-1.0114
C	1.0351	3.2740	-0.1777	H	-6.3271	0.3769	-0.1297				

Table 3.252: Table of thermodynamic data as a function of temperature for 1*H*-Benz[*g*]indeno[2,1-*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.169	409.565	409.565	∞
100	106.710	347.074	762.120	-41.505	436.580	484.834	-253.246
200	207.357	450.204	580.465	-26.052	422.330	538.758	-140.706
250	266.350	502.755	559.644	-14.222	415.592	568.646	-118.810
298.15	324.314	554.631	554.631	0.000	409.565	598.685	-104.885
300	326.521	556.644	554.637	0.602	409.343	599.857	-104.442
350	384.681	611.386	558.827	18.396	403.770	632.062	-94.328
400	438.785	666.337	568.833	39.002	398.920	665.006	-86.839
450	487.894	720.905	582.704	62.190	394.721	698.524	-81.081
500	531.857	774.629	599.219	87.705	391.089	732.498	-76.522
600	605.740	878.393	637.177	144.730	385.232	801.361	-69.763
700	664.366	976.340	678.704	208.345	381.018	871.076	-64.999
800	711.560	1068.244	721.715	277.223	378.248	941.279	-61.458
900	750.158	1154.356	765.054	350.372	376.729	1011.748	-58.719
1000	782.146	1235.100	808.064	427.035	376.286	1082.339	-56.534
1100	808.930	1310.939	850.368	506.628	376.716	1152.939	-54.747
1200	831.538	1382.322	891.753	588.682	377.872	1223.450	-53.254
1300	850.753	1449.659	932.104	672.822	379.569	1293.852	-51.987
1400	867.180	1513.324	971.366	758.740	381.674	1364.111	-50.895
1500	881.302	1573.647	1009.525	846.182	384.102	1434.209	-49.943
1600	893.504	1630.923	1046.588	934.937	386.724	1504.130	-49.104
1700	904.100	1685.417	1082.577	1024.829	389.464	1573.859	-48.358
1800	913.345	1737.362	1117.522	1115.712	392.250	1643.486	-47.692
1900	921.446	1786.965	1151.460	1207.460	395.047	1712.909	-47.090
2000	928.577	1834.415	1184.430	1299.969	397.801	1782.210	-46.546
2100	934.879	1879.876	1216.472	1393.148	400.437	1851.361	-46.049
2200	940.472	1923.498	1247.625	1486.921	402.953	1920.395	-45.595
2300	945.453	1965.415	1277.928	1581.222	405.341	1989.313	-45.178
2400	949.906	2005.749	1307.419	1675.994	407.535	2058.088	-44.792
2500	953.900	2044.609	1336.134	1771.188	409.544	2126.882	-44.438
2600	957.495	2082.093	1364.108	1866.761	411.333	2195.490	-44.107
2700	960.740	2118.291	1391.374	1962.675	412.905	2264.099	-43.801
2800	963.679	2153.285	1417.964	2058.898	414.237	2332.677	-43.516
2900	966.347	2187.149	1443.907	2155.402	415.298	2401.161	-43.249
3000	968.776	2219.951	1469.231	2252.160	416.130	2469.636	-42.999
3100	970.994	2251.754	1493.963	2349.150	416.660	2538.019	-42.764
3200	973.023	2282.614	1518.129	2446.352	416.926	2606.456	-42.545
3300	974.884	2312.584	1541.751	2543.749	416.911	2674.925	-42.340
3400	976.595	2341.713	1564.853	2641.324	416.589	2743.320	-42.145
3500	978.171	2370.045	1587.456	2739.063	415.964	2811.712	-41.962
3600	979.626	2397.622	1609.579	2836.954	415.055	2880.205	-41.790
3700	980.972	2424.481	1631.242	2934.985	413.833	2948.746	-41.628
3800	982.218	2450.659	1652.463	3033.145	412.274	3017.265	-41.474
3900	983.376	2476.188	1673.258	3131.426	410.415	3085.785	-41.329
4000	984.452	2501.098	1693.644	3229.818	408.241	3154.484	-41.192
4100	985.454	2525.420	1713.636	3328.314	405.719	3223.171	-41.063
4200	986.389	2549.178	1733.248	3426.906	402.875	3291.916	-40.940
4300	987.262	2572.398	1752.494	3525.589	399.694	3360.650	-40.823
4400	988.079	2595.105	1771.387	3624.357	396.186	3429.548	-40.713
4500	988.844	2617.318	1789.940	3723.203	392.364	3498.582	-40.610
4600	989.562	2639.060	1808.163	3822.124	388.179	3567.709	-40.512
4700	990.237	2660.349	1826.069	3921.114	383.646	3636.826	-40.418
4800	990.871	2681.203	1843.668	4020.170	378.807	3706.141	-40.330
4900	991.468	2701.641	1860.970	4119.287	373.595	3775.436	-40.246
5000	992.031	2721.677	1877.984	4218.463	368.095	3845.016	-40.168

3.253. 1*H*-Indeno[1,2-*a*]triphenylene



Other names: 3,4-(*o,o'*-Biphenylene)fluorene

Formula: C₂₅H₁₆

Mass: 316.395 g/mol

CAS Number: 188-69-2

Point Group: C₁

Length: 14.11 Å

Width: 10.35 Å

Breadth: 5.686 Å

L/B Ratio: 1.363

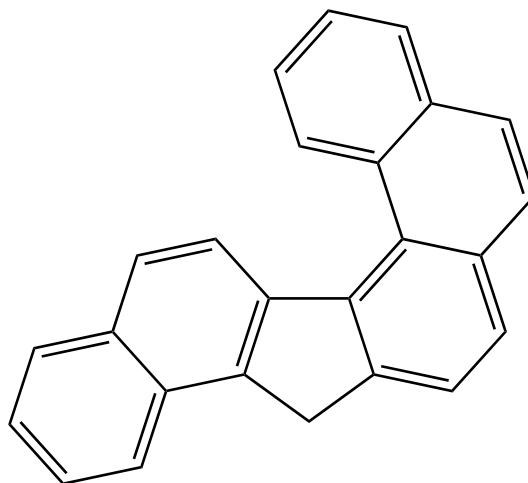
Cartesian coordinates:

C	4.0701	-1.6323	1.0280	C	-2.4163	1.0230	0.0416	H	1.9251	-1.9160	0.9800
C	5.1406	-0.7823	0.7769	C	-3.3795	2.0362	0.1941	H	3.4624	3.0335	0.2477
C	4.9239	0.4998	0.2692	C	-4.6773	1.7328	0.5573	H	3.5046	2.5083	-1.4495
C	2.7598	-1.2455	0.7429	C	-5.0492	0.4036	0.7777	H	0.9725	4.0685	-0.8370
C	2.5354	0.0033	0.1809	C	-4.1227	-0.6067	0.6095	H	-1.4285	3.4550	-0.5024
C	3.6262	0.8883	-0.0059	C	-0.5118	-1.0588	-0.3461	H	-3.0820	3.0824	0.0257
C	3.1356	2.2349	-0.4435	C	-1.8480	-1.3775	-0.0444	H	-5.4156	2.5322	0.6773
C	1.2966	0.7109	-0.1766	C	-2.2711	-2.7165	-0.1010	H	-6.0752	0.1662	1.0768
C	1.6459	2.0535	-0.4375	C	-1.4142	-3.7106	-0.5311	H	-4.4080	-1.6593	0.7589
C	0.6836	3.0361	-0.6177	C	-0.1238	-3.3771	-0.9497	H	-3.3061	-2.9555	0.1881
C	-0.6465	2.6816	-0.4600	C	0.3165	-2.0694	-0.8640	H	-1.7506	-4.7516	-0.5690
C	-0.0518	0.3187	-0.2366	H	4.2537	-2.6210	1.4616	H	0.5369	-4.1525	-1.3510
C	-1.0241	1.3476	-0.2416	H	6.1614	-1.1117	0.9962	H	1.3185	-1.8083	-1.2296
C	-2.8017	-0.3144	0.2289	H	5.7597	1.1873	0.1068				

Table 3.253: Table of thermodynamic data as a function of temperature for 1*H*-Indeno[1,2-*a*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.405	427.598	427.598	∞
100	108.198	347.212	763.802	-41.659	454.458	502.699	-262.578
200	208.115	451.223	581.642	-26.084	440.332	556.556	-145.355
250	266.634	503.889	560.803	-14.228	433.619	586.389	-122.517
298.15	324.314	555.789	555.789	0.000	427.598	616.372	-107.984
300	326.513	557.802	555.795	0.602	427.376	617.543	-107.522
350	384.542	612.532	559.985	18.391	421.799	649.690	-96.959
400	438.611	667.461	569.987	38.990	416.941	682.578	-89.134
450	487.730	722.009	583.854	62.170	412.733	716.039	-83.114
500	531.719	775.717	600.363	87.677	409.094	749.959	-78.346
600	605.640	879.460	638.310	144.690	403.225	818.714	-71.274
700	664.272	977.392	679.827	208.296	399.002	888.324	-66.286
800	711.451	1069.283	722.828	277.164	396.221	958.422	-62.577
900	750.026	1155.380	766.158	350.300	394.690	1028.788	-59.708
1000	781.993	1236.109	809.159	426.949	394.233	1099.277	-57.419
1100	808.760	1311.933	851.455	506.526	394.647	1169.777	-55.547
1200	831.358	1383.300	892.831	588.563	395.785	1240.189	-53.983
1300	850.567	1450.623	933.174	672.685	397.464	1310.494	-52.655
1400	866.994	1514.274	972.428	758.584	399.551	1380.657	-51.512
1500	881.118	1574.584	1010.579	846.007	401.960	1450.661	-50.515
1600	893.324	1631.849	1047.634	934.743	404.564	1520.488	-49.638
1700	903.926	1686.332	1083.616	1024.618	407.287	1590.126	-48.858
1800	913.177	1738.267	1118.554	1115.484	410.055	1659.662	-48.161
1900	921.286	1787.862	1152.485	1207.216	412.836	1728.995	-47.532
2000	928.424	1835.303	1185.449	1299.709	415.574	1798.206	-46.963
2100	934.734	1880.757	1217.484	1392.873	418.195	1867.269	-46.445
2200	940.334	1924.372	1248.631	1486.632	420.697	1936.215	-45.971
2300	945.322	1966.284	1278.928	1580.919	423.072	2005.046	-45.535
2400	949.782	2006.612	1308.413	1675.679	425.253	2073.735	-45.133
2500	953.782	2045.467	1337.123	1770.860	427.250	2142.442	-44.763
2600	957.383	2082.946	1365.092	1866.422	429.027	2210.965	-44.418
2700	960.634	2119.140	1392.353	1962.325	430.589	2279.488	-44.098
2800	963.578	2154.130	1418.938	2058.538	431.910	2347.982	-43.801
2900	966.251	2187.991	1444.877	2155.032	432.961	2416.381	-43.523
3000	968.686	2220.790	1470.197	2251.781	433.784	2484.773	-43.263
3100	970.908	2252.590	1494.925	2348.762	434.305	2553.072	-43.018
3200	972.941	2283.448	1519.086	2445.956	434.563	2621.426	-42.789
3300	974.806	2313.415	1542.705	2543.345	434.540	2689.811	-42.575
3400	976.521	2342.542	1565.803	2640.912	434.210	2758.124	-42.373
3500	978.100	2370.872	1588.402	2738.644	433.578	2826.432	-42.181
3600	979.558	2398.447	1610.522	2836.528	432.661	2894.842	-42.002
3700	980.907	2425.304	1632.182	2934.552	431.434	2963.302	-41.833
3800	982.157	2451.480	1653.400	3032.706	429.868	3031.738	-41.673
3900	983.317	2477.007	1674.192	3130.981	428.003	3100.176	-41.521
4000	984.395	2501.917	1694.575	3229.367	425.823	3168.793	-41.379
4100	985.400	2526.236	1714.564	3327.857	423.296	3237.399	-41.244
4200	986.337	2549.993	1734.173	3426.444	420.446	3306.062	-41.116
4300	987.212	2573.213	1753.417	3525.122	417.260	3374.715	-40.994
4400	988.031	2595.918	1772.308	3623.885	413.747	3443.531	-40.879
4500	988.798	2618.130	1790.858	3722.727	409.920	3512.484	-40.771
4600	989.518	2639.871	1809.079	3821.643	405.731	3581.530	-40.669
4700	990.194	2661.159	1826.983	3920.629	401.193	3650.566	-40.571
4800	990.830	2682.013	1844.579	4019.681	396.351	3719.800	-40.479
4900	991.429	2702.449	1861.879	4118.794	391.134	3789.013	-40.391
5000	991.993	2722.485	1878.892	4217.965	385.631	3858.513	-40.309

3.254. 9H-Benz[4,5]indeno[2,1-c]phenanthrene



Formula: C₂₅H₁₆
Mass: 316.395 g/mol
CAS Number: 192-77-8
Point Group: C₁

Length: 14.70 Å
Width: 10.21 Å
Breadth: 5.374 Å
L/B Ratio: 1.440

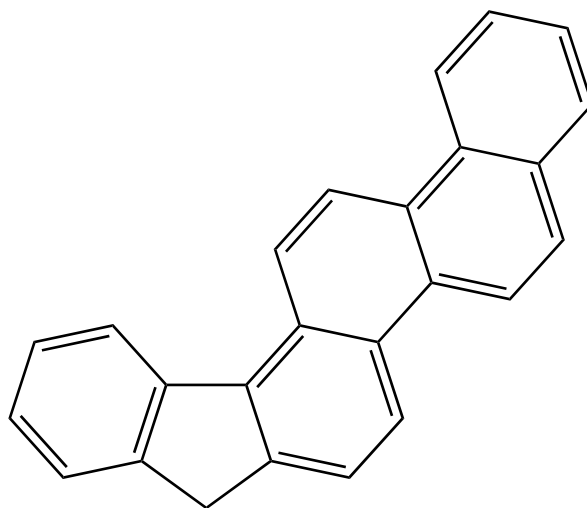
Cartesian coordinates:

C	-4.5998	1.7843	-0.4376	C	2.0642	-3.1137	-0.0377	H	-4.3429	-1.9509	0.6472
C	-5.7302	1.0715	-0.1454	C	1.7698	-0.6705	0.0031	H	0.0023	1.8663	-0.8519
C	-5.6420	-0.2855	0.2476	C	2.5873	-1.8119	-0.1762	H	-2.2343	2.9220	-1.0306
C	-4.4246	-0.9010	0.3438	C	3.9708	-1.6495	-0.5367	H	-1.9025	-2.5102	1.4322
C	-3.3196	1.1717	-0.3473	C	4.5250	-0.4199	-0.6320	H	-2.1007	-2.8785	-0.2957
C	-3.2338	-0.1812	0.0533	C	2.4302	0.6119	0.1506	H	0.3188	-4.3134	0.3992
C	-0.8989	1.3129	-0.5607	C	3.7789	0.7417	-0.2339	H	2.7364	-3.9732	-0.1421
C	-2.1382	1.8898	-0.6739	C	4.4214	1.9940	-0.1440	H	4.5555	-2.5500	-0.7580
C	-0.7936	-0.0157	-0.0996	C	3.7629	3.0756	0.3965	H	5.5612	-0.2867	-0.9627
C	-1.9489	-0.7606	0.1419	C	2.4599	2.9217	0.8925	H	5.4556	2.0906	-0.4936
C	-1.6025	-2.1935	0.4155	C	1.8095	1.7123	0.7777	H	4.2580	4.0495	0.4650
C	0.3767	-0.8911	0.0639	H	-4.6621	2.8342	-0.7454	H	1.9641	3.7675	1.3800
C	-0.1105	-2.1970	0.2569	H	-6.7171	1.5409	-0.2129	H	0.8072	1.5878	1.2084
C	0.7265	-3.3107	0.2385	H	-6.5624	-0.8338	0.4734				

Table 3.254: Table of thermodynamic data as a function of temperature for 9*H*-Benz[4,5]indeno[2,1-*c*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-47.909	423.688	423.688	∞
100	105.868	342.865	756.691	-41.383	450.824	499.500	-260.906
200	206.808	445.538	575.510	-25.994	436.511	553.872	-144.654
250	265.765	497.964	554.734	-14.193	429.745	583.996	-122.017
298.15	323.665	549.731	549.731	0.000	423.688	614.268	-107.615
300	325.870	551.740	549.737	0.601	423.465	615.450	-107.157
350	383.987	606.379	553.920	18.361	417.858	647.903	-96.692
400	438.082	661.236	563.907	38.932	412.973	681.100	-88.941
450	487.211	715.722	577.754	62.086	408.739	714.874	-82.979
500	531.211	769.376	594.242	87.567	405.074	749.109	-78.257
600	605.186	873.030	632.144	144.532	399.157	818.503	-71.256
700	663.904	970.899	673.619	208.096	394.892	888.759	-66.319
800	711.175	1062.747	716.581	276.932	392.079	959.509	-62.648
900	749.836	1148.817	759.877	350.045	390.525	1030.530	-59.809
1000	781.875	1229.529	802.850	426.680	390.053	1101.676	-57.544
1100	808.698	1305.345	845.120	506.247	390.458	1172.834	-55.692
1200	831.339	1376.709	886.475	588.280	391.592	1243.906	-54.145
1300	850.579	1444.031	926.799	672.402	393.271	1314.870	-52.831
1400	867.028	1507.684	966.039	758.303	395.360	1385.692	-51.700
1500	881.168	1567.997	1004.177	845.730	397.773	1456.355	-50.714
1600	893.385	1625.265	1041.220	934.473	400.383	1526.841	-49.845
1700	903.994	1679.752	1077.191	1024.354	403.112	1597.137	-49.073
1800	913.249	1731.691	1112.121	1115.226	405.887	1667.331	-48.384
1900	921.360	1781.290	1146.045	1206.965	408.676	1737.321	-47.761
2000	928.498	1828.735	1179.002	1299.466	411.421	1807.189	-47.198
2100	934.808	1874.192	1211.032	1392.638	414.050	1876.909	-46.685
2200	940.406	1917.811	1242.173	1486.404	416.559	1946.511	-46.215
2300	945.393	1959.726	1272.466	1580.698	418.940	2015.998	-45.784
2400	949.850	2000.058	1301.947	1675.465	421.129	2085.342	-45.385
2500	953.849	2038.915	1330.654	1770.653	423.132	2154.705	-45.019
2600	957.447	2076.397	1358.620	1866.221	424.916	2223.883	-44.677
2700	960.696	2112.593	1385.878	1962.131	426.484	2293.061	-44.361
2800	963.637	2147.585	1412.460	2058.350	427.811	2362.209	-44.067
2900	966.308	2181.448	1438.397	2154.850	428.869	2431.263	-43.791
3000	968.740	2214.249	1463.714	2251.604	429.697	2500.309	-43.533
3100	970.960	2246.051	1488.441	2348.591	430.224	2569.262	-43.291
3200	972.991	2276.910	1512.601	2445.790	430.487	2638.269	-43.064
3300	974.854	2306.879	1536.218	2543.183	430.468	2707.308	-42.852
3400	976.567	2336.007	1559.315	2640.755	430.143	2776.274	-42.651
3500	978.145	2364.339	1581.913	2738.492	429.515	2845.237	-42.462
3600	979.601	2391.915	1604.031	2836.380	428.603	2914.300	-42.285
3700	980.948	2418.773	1625.690	2934.409	427.380	2983.412	-42.117
3800	982.196	2444.950	1646.906	3032.567	425.818	3052.502	-41.959
3900	983.354	2470.478	1667.698	3130.845	423.957	3121.593	-41.808
4000	984.431	2495.389	1688.080	3229.235	421.781	3190.862	-41.668
4100	985.434	2519.709	1708.068	3327.728	419.257	3260.121	-41.534
4200	986.370	2543.467	1727.677	3426.319	416.410	3329.437	-41.407
4300	987.244	2566.687	1746.920	3525.000	413.227	3398.742	-41.286
4400	988.062	2589.393	1765.810	3623.766	409.718	3468.211	-41.172
4500	988.828	2611.606	1784.359	3722.611	405.894	3537.817	-41.065
4600	989.547	2633.348	1802.580	3821.530	401.708	3607.515	-40.964
4700	990.222	2654.636	1820.483	3920.519	397.173	3677.203	-40.867
4800	990.857	2675.491	1838.079	4019.573	392.333	3747.089	-40.776
4900	991.454	2695.928	1855.379	4118.689	387.119	3816.955	-40.688
5000	992.018	2715.963	1872.391	4217.863	381.618	3887.107	-40.607

3.255. 5*H*-Indeno[2,1-*a*]chrysene



Formula: C₂₅H₁₆
Mass: 316.395 g/mol
Point Group: C_s

Length: 16.58 Å
Width: 9.634 Å
Breadth: 4.177 Å
L/B Ratio: 1.721

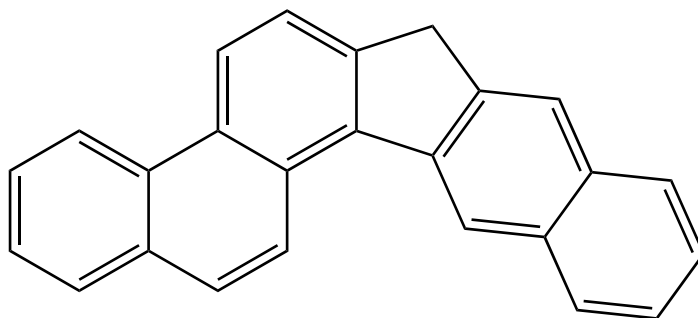
Cartesian coordinates:

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C	-2.1786	-0.2871	0.0019	C	-0.7852	-0.0544	0.0019	H	6.3715	-1.2522	-0.0030
C	-2.6726	-1.5974	0.0017	C	0.0794	-1.1746	0.0002	H	3.3323	2.7022	0.0038
C	5.3743	2.0098	0.0020	C	-0.4589	-2.4831	-0.0009	H	4.4415	-2.7481	-0.0044
C	6.2324	0.8927	0.0001	C	-1.8179	-2.7024	0.0001	H	1.9838	-3.0917	-0.0038
C	5.7114	-0.3774	-0.0015	C	-3.3271	0.6272	0.0007	H	-0.8932	2.1253	0.0064
C	4.0127	1.8371	0.0023	C	-4.5117	-0.1512	-0.0006	H	1.5616	2.4526	0.0045
C	3.4489	0.5381	0.0007	C	-5.7598	0.4426	-0.0032	H	0.2358	-3.3368	-0.0028
C	4.3097	-0.5747	-0.0012	C	-5.8330	1.8368	-0.0046	H	-2.2294	-3.7165	-0.0005
C	3.7565	-1.8926	-0.0028	C	-4.6761	2.6071	-0.0026	H	-6.6691	-0.1663	-0.0042
C	2.4107	-2.0773	-0.0024	C	-3.4144	2.0111	0.0005	H	-6.8125	2.3260	-0.0073
C	2.0237	0.3294	0.0011	H	-4.5808	-2.1296	0.8885	H	-4.7533	3.6995	-0.0031
C	1.5082	-0.9672	-0.0003	H	-4.5775	-2.1303	-0.8889	H	-2.5109	2.6344	0.0040
C	-0.2187	1.2582	0.0038	H	5.8043	3.0166	0.0033				

Table 3.255: Table of thermodynamic data as a function of temperature for 5*H*-Indeno[2,1-*a*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.023	399.333	399.333	∞
100	109.905	362.120	781.308	-41.919	425.933	472.683	-246.899
200	209.387	467.034	598.112	-26.216	411.935	524.997	-137.112
250	268.004	519.998	577.172	-14.293	405.289	554.032	-115.756
298.15	325.624	572.135	572.135	0.000	399.333	583.234	-102.178
300	327.818	574.156	572.141	0.604	399.114	584.373	-101.746
350	385.670	629.075	576.346	18.455	393.597	615.698	-91.886
400	439.525	684.141	586.381	39.104	388.790	647.755	-84.586
450	488.439	738.784	600.285	62.325	384.623	680.380	-78.975
500	532.251	792.558	616.832	87.863	381.015	713.459	-74.533
600	605.915	896.373	654.847	144.915	375.185	780.526	-67.949
700	664.391	994.335	696.421	208.540	370.981	848.443	-63.310
800	711.478	1086.235	739.466	277.415	368.207	916.846	-59.863
900	750.001	1172.332	782.831	350.551	366.676	985.517	-57.197
1000	781.938	1253.057	825.860	427.196	366.215	1054.311	-55.070
1100	808.689	1328.875	868.178	506.766	366.622	1123.116	-53.331
1200	831.279	1400.235	909.572	588.796	367.753	1191.834	-51.878
1300	850.486	1467.552	949.929	672.910	369.424	1260.446	-50.644
1400	866.912	1531.197	989.196	758.800	371.503	1328.917	-49.581
1500	881.038	1591.501	1027.357	846.215	373.904	1397.229	-48.655
1600	893.248	1648.761	1064.421	934.944	376.499	1465.365	-47.838
1700	903.853	1703.240	1100.409	1024.812	379.215	1533.311	-47.112
1800	913.108	1755.170	1135.354	1115.670	381.976	1601.157	-46.463
1900	921.221	1804.762	1169.290	1207.395	384.750	1668.800	-45.878
2000	928.363	1852.200	1202.259	1299.882	387.482	1736.321	-45.347
2100	934.676	1897.650	1234.298	1393.040	390.097	1803.695	-44.864
2200	940.279	1941.263	1265.448	1486.793	392.594	1870.951	-44.421
2300	945.271	1983.173	1295.748	1581.076	394.963	1938.093	-44.015
2400	949.733	2023.499	1325.237	1675.830	397.139	2005.093	-43.639
2500	953.737	2062.352	1353.949	1771.007	399.131	2072.112	-43.294
2600	957.340	2099.829	1381.920	1866.564	400.904	2138.946	-42.971
2700	960.594	2136.022	1409.183	1962.463	402.462	2205.782	-42.673
2800	963.540	2171.010	1435.770	2058.672	403.779	2272.587	-42.395
2900	966.215	2204.870	1461.710	2155.162	404.827	2339.299	-42.134
3000	968.651	2237.668	1487.032	2251.908	405.646	2406.002	-41.891
3100	970.875	2269.466	1511.761	2348.886	406.164	2472.614	-41.662
3200	972.910	2300.323	1535.924	2446.076	406.418	2539.280	-41.449
3300	974.777	2330.290	1559.544	2543.462	406.392	2605.978	-41.248
3400	976.493	2359.416	1582.643	2641.027	406.060	2672.603	-41.059
3500	978.074	2387.745	1605.243	2738.756	405.424	2739.224	-40.880
3600	979.533	2415.319	1627.364	2836.637	404.506	2805.947	-40.712
3700	980.883	2442.176	1649.025	2934.659	403.275	2872.719	-40.555
3800	982.134	2468.351	1670.243	3032.811	401.707	2939.468	-40.405
3900	983.295	2493.878	1691.036	3131.083	399.840	3006.219	-40.263
4000	984.374	2518.786	1711.420	3229.467	397.658	3073.149	-40.130
4100	985.380	2543.106	1731.409	3327.955	395.128	3140.068	-40.004
4200	986.318	2566.862	1751.019	3426.541	392.277	3207.045	-39.885
4300	987.194	2590.081	1770.263	3525.217	389.089	3274.010	-39.771
4400	988.014	2612.786	1789.154	3623.978	385.575	3341.140	-39.664
4500	988.782	2634.998	1807.705	3722.818	381.746	3408.406	-39.563
4600	989.502	2656.738	1825.927	3821.732	377.555	3475.765	-39.468
4700	990.179	2678.026	1843.831	3920.717	373.016	3543.114	-39.376
4800	990.815	2698.879	1861.428	4019.767	368.172	3610.661	-39.291
4900	991.414	2719.315	1878.728	4118.878	362.954	3678.188	-39.209
5000	991.979	2739.350	1895.741	4218.048	357.449	3746.001	-39.133

3.256. 7H-Benz[5,6]indeno[1,2-a]phenanthrene



Formula: C₂₅H₁₆
Mass: 316.395 g/mol
CAS Number: 908070-09-7
Point Group: C_s

Length: 16.78 Å
Width: 9.601 Å
Breadth: 4.176 Å
L/B Ratio: 1.748

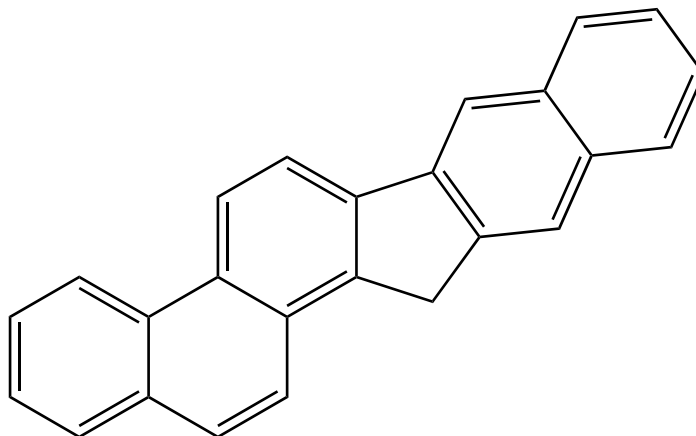
Cartesian coordinates:

C	5.4956	-2.2222	0.0000	C	-2.4300	2.1229	0.0000	H	3.5268	-3.0779	0.0000
C	6.2639	-1.0366	-0.0000	C	-1.1744	0.0200	0.0000	H	4.1809	2.4634	-0.0000
C	5.6487	0.1872	-0.0000	C	-2.4074	0.7134	0.0000	H	1.4640	-1.7732	0.0000
C	4.1274	-2.1613	0.0000	C	-2.3405	-2.1161	0.0000	H	1.4893	3.4264	0.8884
C	3.4637	-0.9055	0.0000	C	-1.1823	-1.4165	0.0000	H	1.4893	3.4264	-0.8884
C	4.2322	0.2782	0.0000	C	-3.6080	-1.4422	0.0000	H	-1.2846	3.9541	0.0000
C	3.5815	1.5467	0.0000	C	-3.6471	-0.0374	0.0000	H	-3.4061	2.6322	0.0000
C	2.0401	-0.8377	0.0000	C	-4.9030	0.6074	0.0000	H	-2.3364	-3.2123	0.0000
C	1.4285	0.3842	0.0000	C	-6.0691	-0.1237	-0.0000	H	-0.2194	-1.9449	0.0000
C	2.2203	1.5866	0.0000	C	-6.0243	-1.5272	-0.0000	H	-4.9304	1.7076	0.0000
C	1.3243	2.7889	0.0000	C	-4.8118	-2.1786	0.0000	H	-7.0386	0.3850	-0.0000
C	0.0137	0.7778	0.0000	H	6.0086	-3.1894	0.0000	H	-6.9591	-2.0971	-0.0000
C	-0.0470	2.1799	0.0000	H	7.3563	-1.1095	-0.0000	H	-4.7686	-3.2736	0.0000
C	-1.2631	2.8599	0.0000	H	6.2385	1.1108	-0.0000				

Table 3.256: Table of thermodynamic data as a function of temperature for 7*H*-Benz[5,6]indeno[1,2-*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.691	396.148	396.148	∞
100	108.398	357.709	775.344	-41.764	422.904	470.095	-245.547
200	208.665	461.875	592.694	-26.164	408.802	522.896	-136.564
250	267.487	514.700	571.790	-14.272	402.125	552.192	-115.372
298.15	325.260	566.760	566.760	0.000	396.148	581.651	-101.901
300	327.459	568.779	566.767	0.604	395.928	582.801	-101.473
350	385.421	623.652	570.968	18.439	390.397	614.396	-91.692
400	439.349	678.690	580.995	39.078	385.580	646.725	-84.452
450	488.312	733.315	594.891	62.291	381.404	679.623	-78.887
500	532.160	787.077	611.430	87.824	377.791	712.976	-74.483
600	605.880	890.881	649.431	144.870	371.956	780.592	-67.955
700	664.407	988.842	690.993	208.494	367.750	849.057	-63.356
800	711.539	1080.747	734.031	277.373	364.980	918.010	-59.939
900	750.099	1166.853	777.390	350.517	363.457	987.229	-57.296
1000	782.063	1247.590	820.416	427.173	363.007	1056.570	-55.188
1100	808.833	1323.420	862.732	506.757	363.428	1125.922	-53.464
1200	831.435	1394.794	904.126	588.801	364.574	1195.185	-52.024
1300	850.646	1462.123	944.484	672.931	366.260	1264.340	-50.801
1400	867.074	1525.780	983.753	758.838	368.355	1333.353	-49.747
1500	881.198	1586.096	1021.916	846.269	370.772	1402.206	-48.828
1600	893.404	1643.366	1058.982	935.014	373.384	1470.882	-48.018
1700	904.004	1697.854	1094.973	1024.896	376.115	1539.368	-47.298
1800	913.253	1749.793	1129.921	1115.770	378.891	1607.751	-46.655
1900	921.359	1799.392	1163.861	1207.509	381.679	1675.931	-46.074
2000	928.494	1846.836	1196.832	1300.009	384.424	1743.990	-45.547
2100	934.801	1892.294	1228.874	1393.180	387.053	1811.899	-45.068
2200	940.398	1935.912	1260.028	1486.946	389.561	1879.691	-44.629
2300	945.383	1977.827	1290.331	1581.239	391.942	1947.368	-44.225
2400	949.840	2018.158	1319.822	1676.005	394.129	2014.903	-43.852
2500	953.838	2057.015	1348.538	1771.192	396.132	2082.455	-43.510
2600	957.436	2094.496	1376.512	1866.759	397.914	2149.823	-43.190
2700	960.684	2130.692	1403.778	1962.668	399.481	2217.191	-42.893
2800	963.626	2165.684	1430.368	2058.886	400.807	2284.530	-42.618
2900	966.297	2199.546	1456.310	2155.384	401.863	2351.774	-42.359
3000	968.729	2232.347	1481.634	2252.137	402.690	2419.009	-42.118
3100	970.949	2264.148	1506.366	2349.122	403.216	2486.153	-41.891
3200	972.980	2295.007	1530.532	2446.320	403.478	2553.351	-41.678
3300	974.844	2324.976	1554.154	2543.713	403.458	2620.580	-41.479
3400	976.557	2354.104	1577.255	2641.284	403.133	2687.736	-41.291
3500	978.134	2382.435	1599.858	2739.020	402.503	2754.889	-41.114
3600	979.591	2410.010	1621.981	2836.907	401.590	2822.143	-40.947
3700	980.938	2436.869	1643.643	2934.934	400.366	2889.446	-40.791
3800	982.186	2463.045	1664.863	3033.091	398.803	2956.726	-40.642
3900	983.345	2488.573	1685.658	3131.369	396.941	3024.007	-40.501
4000	984.423	2513.483	1706.044	3229.758	394.764	3091.467	-40.370
4100	985.426	2537.804	1726.035	3328.251	392.239	3158.916	-40.244
4200	986.362	2561.561	1745.647	3426.841	389.392	3226.423	-40.126
4300	987.236	2584.781	1764.893	3525.521	386.208	3293.919	-40.012
4400	988.054	2607.487	1783.786	3624.286	382.698	3361.578	-39.906
4500	988.821	2629.700	1802.338	3723.130	378.874	3429.374	-39.806
4600	989.540	2651.441	1820.561	3822.049	374.687	3497.263	-39.712
4700	990.215	2672.730	1838.467	3921.037	370.151	3565.142	-39.621
4800	990.850	2693.584	1856.065	4020.090	365.311	3633.219	-39.537
4900	991.448	2714.021	1873.366	4119.205	360.096	3701.275	-39.455
5000	992.011	2734.056	1890.381	4218.379	354.594	3769.618	-39.380

3.257. 7H-Benz[5,6]indeno[2,1-a]phenanthrene



Formula: C₂₅H₁₆
Mass: 316.395 g/mol
Point Group: C_s

Length: 17.93 Å
Width: 7.966 Å
Breadth: 4.176 Å
L/B Ratio: 2.251

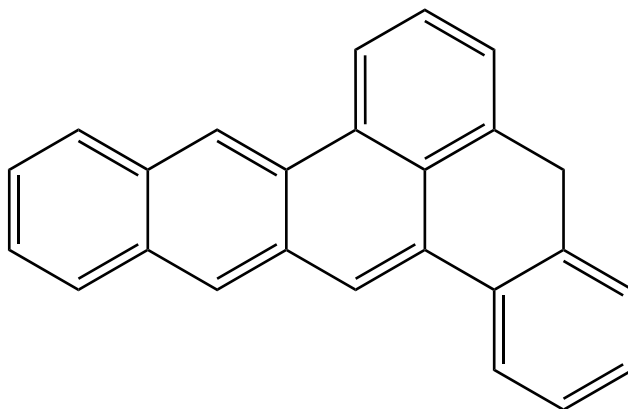
Cartesian coordinates:

C	2.0436	1.0381	-0.0000	C	-0.3609	-1.7880	0.0000	H	7.8284	0.6153	0.0000
C	0.7287	1.7657	-0.0000	C	-2.4139	-0.4772	0.0000	H	5.9150	2.2003	0.0000
C	1.8128	-0.3808	0.0000	C	-1.6777	0.7282	0.0000	H	5.1094	-2.7237	0.0000
C	6.5707	-1.1506	0.0000	C	-2.3653	1.9897	0.0000	H	3.4965	2.6217	-0.0000
C	6.7985	0.2435	0.0000	C	-3.7172	2.0427	0.0000	H	2.6766	-2.3500	0.0000
C	5.7441	1.1178	0.0000	C	-3.8608	-0.4143	0.0000	H	-2.3443	-2.6368	-0.0000
C	5.2927	-1.6433	0.0000	C	-4.5008	0.8377	0.0000	H	0.1590	-2.7517	0.0000
C	4.1814	-0.7595	0.0000	C	-5.9103	0.9016	0.0000	H	-1.7605	2.9042	0.0000
C	4.4094	0.6345	0.0000	C	-6.6590	-0.2537	0.0000	H	-4.2446	3.0036	0.0000
C	3.3083	1.5428	-0.0000	C	-6.0233	-1.5057	-0.0000	H	-6.4011	1.8816	0.0000
C	2.8493	-1.2680	0.0000	C	-4.6492	-1.5849	-0.0000	H	-7.7527	-0.2041	0.0000
C	0.3674	-0.5962	0.0000	H	0.6180	2.4150	0.8886	H	-6.6283	-2.4182	-0.0000
C	-0.2775	0.6474	-0.0000	H	0.6180	2.4150	-0.8886	H	-4.1390	-2.5603	-0.0000
C	-1.7398	-1.7165	-0.0000	H	7.4285	-1.8310	0.0000				

Table 3.257: Table of thermodynamic data as a function of temperature for 7*H*-Benz[5,6]indeno[2,1-*a*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.345	383.977	383.977	∞
100	107.580	350.265	766.057	-41.579	410.917	458.852	-239.675
200	207.722	453.847	584.170	-26.065	396.730	512.429	-133.830
250	266.468	506.453	563.343	-14.222	390.004	542.133	-113.270
298.15	324.208	558.331	558.331	0.000	383.977	571.993	-100.209
300	326.406	560.343	558.337	0.602	383.755	573.159	-99.794
350	384.371	615.053	562.525	18.385	378.171	605.180	-90.316
400	438.331	669.953	572.524	38.972	373.302	637.942	-83.305
450	487.347	724.461	586.383	62.135	369.077	671.280	-77.919
500	531.261	778.125	602.883	87.621	365.417	705.078	-73.657
600	605.134	881.778	640.803	144.585	359.499	773.597	-67.346
700	663.814	979.635	682.289	208.142	355.227	842.979	-62.903
800	711.083	1071.470	725.259	276.969	352.405	912.856	-59.602
900	749.757	1157.530	768.560	350.073	350.842	983.005	-57.051
1000	781.813	1238.235	811.535	426.700	350.362	1053.280	-55.017
1100	808.654	1314.045	853.807	506.262	350.762	1123.568	-53.353
1200	831.310	1385.406	895.163	588.292	351.893	1193.770	-51.962
1300	850.562	1452.727	935.488	672.411	353.569	1263.864	-50.782
1400	867.021	1516.378	974.728	758.311	355.657	1333.817	-49.764
1500	881.168	1576.691	1012.866	845.738	358.070	1403.610	-48.877
1600	893.391	1633.960	1049.910	934.481	360.680	1473.227	-48.095
1700	904.004	1688.447	1085.881	1024.363	363.410	1542.653	-47.399
1800	913.262	1740.387	1120.811	1115.236	366.186	1611.977	-46.777
1900	921.374	1789.986	1154.735	1206.977	368.976	1681.098	-46.216
2000	928.514	1837.432	1187.693	1299.479	371.723	1750.097	-45.707
2100	934.825	1882.890	1219.723	1392.652	374.353	1818.947	-45.243
2200	940.423	1926.510	1250.865	1486.420	376.864	1887.679	-44.818
2300	945.410	1968.426	1281.158	1580.716	379.247	1956.296	-44.428
2400	949.868	2008.758	1310.639	1675.484	381.437	2024.770	-44.067
2500	953.866	2047.616	1339.346	1770.675	383.443	2093.263	-43.735
2600	957.464	2085.099	1367.312	1866.244	385.228	2161.570	-43.426
2700	960.712	2121.296	1394.571	1962.156	386.798	2229.879	-43.139
2800	963.653	2156.288	1421.154	2058.376	388.127	2298.157	-42.872
2900	966.324	2190.152	1447.090	2154.877	389.186	2366.340	-42.622
3000	968.755	2222.953	1472.409	2251.633	390.015	2434.515	-42.388
3100	970.975	2254.755	1497.135	2348.621	390.544	2502.598	-42.168
3200	973.005	2285.615	1521.296	2445.822	390.808	2570.735	-41.962
3300	974.868	2315.585	1544.913	2543.217	390.791	2638.904	-41.769
3400	976.580	2344.713	1568.010	2640.790	390.468	2706.999	-41.587
3500	978.157	2373.045	1590.608	2738.528	389.841	2775.091	-41.415
3600	979.613	2400.621	1612.727	2836.418	388.930	2843.283	-41.254
3700	980.959	2427.480	1634.386	2934.447	387.707	2911.525	-41.103
3800	982.207	2453.657	1655.603	3032.606	386.147	2979.744	-40.959
3900	983.365	2479.186	1676.395	3130.886	384.287	3047.964	-40.822
4000	984.442	2504.096	1696.777	3229.277	382.112	3116.363	-40.695
4100	985.444	2528.417	1716.766	3327.772	379.589	3184.751	-40.573
4200	986.380	2552.175	1736.375	3426.363	376.744	3253.196	-40.459
4300	987.254	2575.396	1755.618	3525.046	373.562	3321.630	-40.349
4400	988.071	2598.102	1774.508	3623.812	370.053	3390.228	-40.246
4500	988.837	2620.315	1793.058	3722.658	366.230	3458.963	-40.150
4600	989.555	2642.057	1811.279	3821.578	362.045	3527.790	-40.058
4700	990.230	2663.345	1829.182	3920.568	357.511	3596.608	-39.971
4800	990.864	2684.200	1846.779	4019.623	352.672	3665.623	-39.889
4900	991.462	2704.637	1864.078	4118.739	347.458	3734.618	-39.811
5000	992.025	2724.673	1881.090	4217.914	341.958	3803.898	-39.738

3.258. 4*H*-Dibenzo[*a,de*]naphthacene



Other names: Benzanthreno-Bz-1,Bz-2:2,3-naphthalene

Formula: C₂₅H₁₆

Mass: 316.395 g/mol

CAS Number: 198-40-3

Point Group: C_s

Length: 16.04 Å

Width: 10.81 Å

Breadth: 4.171 Å

L/B Ratio: 1.484

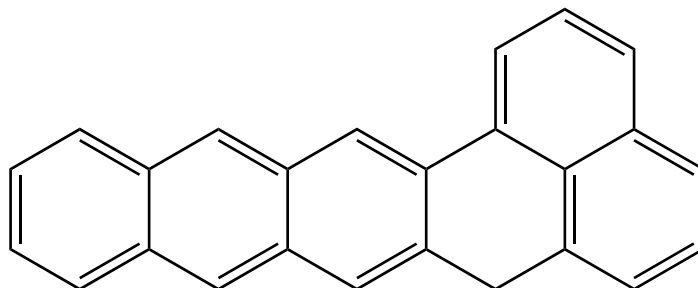
Cartesian coordinates:

C	6.0657	0.1382	0.0000	C	-2.2859	-1.8479	0.0000	H	5.1726	-1.8117	-0.0000
C	5.8457	1.5417	0.0000	C	-2.0848	-3.2219	0.0000	H	1.9690	2.7419	0.0000
C	4.5780	2.0438	0.0000	C	-0.7921	-3.7485	-0.0000	H	2.7373	-2.1975	-0.0000
C	5.0122	-0.7277	0.0000	C	0.2978	-2.9017	-0.0000	H	-0.4343	2.3847	-0.0000
C	3.6724	-0.2342	-0.0000	C	0.1213	-1.5072	-0.0000	H	-4.2163	-1.7550	-0.8858
C	3.4531	1.1641	0.0000	C	-3.8374	0.1385	0.0000	H	-4.2163	-1.7550	0.8858
C	2.1366	1.6578	-0.0000	C	-2.7339	0.9998	0.0000	H	-2.9468	-3.8986	0.0000
C	2.5710	-1.1082	-0.0000	C	-2.9539	2.3842	-0.0000	H	-0.6473	-4.8337	-0.0000
C	1.2729	-0.6194	-0.0000	C	-4.2401	2.9010	-0.0000	H	1.3222	-3.3046	-0.0000
C	1.0558	0.7866	-0.0000	C	-5.3343	2.0400	-0.0000	H	-2.0860	3.0614	-0.0000
C	-0.2911	1.2917	-0.0000	C	-5.1317	0.6677	0.0000	H	-4.3948	3.9847	-0.0000
C	-1.3700	0.4648	0.0000	H	7.0951	-0.2346	0.0000	H	-6.3515	2.4447	-0.0000
C	-3.6880	-1.3432	0.0000	H	6.7118	2.2115	0.0000	H	-5.9912	-0.0124	0.0000
C	-1.1816	-0.9728	0.0000	H	4.3991	3.1250	0.0000				

Table 3.258: Table of thermodynamic data as a function of temperature for 4*H*-Dibenzo[*a,de*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.312	395.823	395.823	∞
100	107.472	350.603	766.057	-41.545	422.797	470.698	-245.862
200	207.623	454.171	584.335	-26.033	408.608	524.243	-136.915
250	266.136	506.731	563.536	-14.201	401.871	553.931	-115.735
298.15	323.668	558.531	558.531	0.000	395.823	583.780	-102.274
300	325.860	560.540	558.537	0.601	395.600	584.945	-101.846
350	383.683	615.154	562.718	18.352	389.985	616.959	-92.074
400	437.574	669.956	572.699	38.903	385.079	649.718	-84.843
450	486.577	724.374	586.534	62.028	380.816	683.058	-79.286
500	530.513	777.958	603.006	87.476	377.118	716.862	-74.889
600	604.482	881.483	640.867	144.370	371.130	785.405	-68.374
700	663.272	979.248	682.295	207.867	366.798	854.821	-63.786
800	710.641	1071.017	725.211	276.645	363.927	924.740	-60.378
900	749.397	1157.030	768.464	349.709	362.324	994.937	-57.743
1000	781.519	1237.700	811.397	426.303	361.812	1065.264	-55.643
1100	808.412	1313.485	853.632	505.839	362.185	1135.607	-53.924
1200	831.109	1384.827	894.955	587.846	363.294	1205.865	-52.489
1300	850.394	1452.133	935.251	671.947	364.951	1276.019	-51.270
1400	866.878	1515.773	974.465	757.832	367.024	1346.032	-50.220
1500	881.046	1576.077	1012.580	845.246	369.424	1415.886	-49.305
1600	893.285	1633.338	1049.603	933.977	372.022	1485.564	-48.498
1700	903.912	1687.820	1085.556	1023.849	374.742	1555.053	-47.780
1800	913.181	1739.754	1120.469	1114.714	377.510	1624.440	-47.139
1900	921.303	1789.350	1154.378	1206.447	380.292	1693.624	-46.560
2000	928.451	1836.792	1187.321	1298.942	383.032	1762.687	-46.036
2100	934.768	1882.247	1219.338	1392.109	385.657	1831.601	-45.558
2200	940.372	1925.864	1250.468	1485.872	388.162	1900.397	-45.120
2300	945.364	1967.778	1280.750	1580.163	390.541	1969.080	-44.718
2400	949.826	2008.108	1310.222	1674.927	392.726	2037.619	-44.347
2500	953.828	2046.965	1338.919	1770.113	394.728	2106.176	-44.005
2600	957.429	2084.446	1366.877	1865.679	396.510	2174.549	-43.686
2700	960.680	2120.641	1394.128	1961.588	398.076	2242.923	-43.391
2800	963.624	2155.633	1420.703	2057.805	399.402	2311.266	-43.116
2900	966.296	2189.495	1446.632	2154.303	400.458	2379.515	-42.859
3000	968.730	2222.296	1471.944	2251.056	401.285	2447.756	-42.618
3100	970.951	2254.097	1496.664	2348.042	401.811	2515.904	-42.392
3200	972.983	2284.956	1520.819	2445.240	402.073	2584.107	-42.180
3300	974.847	2314.925	1544.431	2542.633	402.054	2652.342	-41.982
3400	976.561	2344.053	1567.523	2640.205	401.728	2720.503	-41.795
3500	978.139	2372.384	1590.116	2737.941	401.099	2788.661	-41.618
3600	979.596	2399.960	1612.230	2835.829	400.187	2856.920	-41.452
3700	980.943	2426.819	1633.885	2933.856	398.963	2925.227	-41.296
3800	982.192	2452.996	1655.097	3032.014	397.400	2993.512	-41.148
3900	983.351	2478.524	1675.885	3130.292	395.539	3061.799	-41.007
4000	984.428	2503.434	1696.263	3228.681	393.363	3130.264	-40.876
4100	985.432	2527.754	1716.248	3327.175	390.838	3198.718	-40.751
4200	986.368	2551.512	1735.854	3425.765	387.992	3267.230	-40.633
4300	987.242	2574.732	1755.094	3524.446	384.809	3335.730	-40.520
4400	988.060	2597.438	1773.981	3623.212	381.299	3404.395	-40.414
4500	988.826	2619.651	1792.527	3722.057	377.475	3473.196	-40.315
4600	989.545	2641.392	1810.746	3820.975	373.289	3542.089	-40.221
4700	990.220	2662.681	1828.646	3919.964	368.753	3610.973	-40.131
4800	990.855	2683.535	1846.240	4019.018	363.914	3680.055	-40.046
4900	991.453	2703.972	1863.537	4118.134	358.699	3749.116	-39.965
5000	992.017	2724.008	1880.546	4217.308	353.198	3818.463	-39.890

3.259. 7H-Benzo[de]pentacene



Formula: $C_{25}H_{16}$
Mass: 316.395 g/mol
CAS Number: 229-15-2
Point Group: C_s

Length: 16.76 Å
Width: 9.591 Å
Breadth: 4.171 Å
L/B Ratio: 1.748

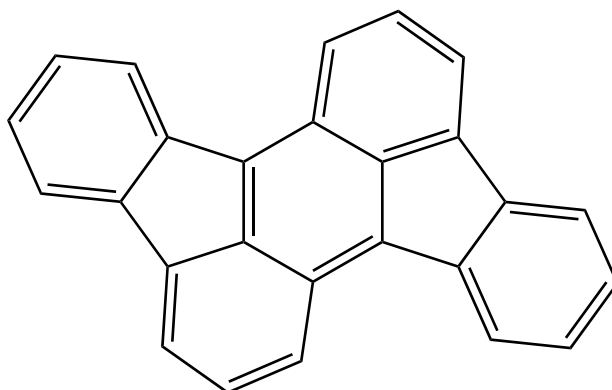
Cartesian coordinates:

C	6.4839	-0.9420	0.0000	C	-1.8363	2.0409	0.0000	H	5.1453	-2.6141	0.0000
C	6.6138	0.4777	0.0000	C	-3.1639	1.3655	0.0000	H	3.1541	2.5907	-0.0000
C	5.5108	1.2728	-0.0000	C	-4.3028	2.1388	0.0000	H	2.6982	-2.3918	0.0000
C	5.2551	-1.5237	0.0000	C	-5.5808	1.5423	0.0000	H	0.7069	2.8068	0.0000
C	4.0685	-0.7192	0.0000	C	-5.7070	0.1794	0.0000	H	0.2485	-2.1654	0.0000
C	4.1980	0.6971	0.0000	C	-3.2693	-0.0525	0.0000	H	-1.7784	2.7083	0.8858
C	3.0546	1.4983	-0.0000	C	-4.5508	-0.6448	0.0000	H	-1.7784	2.7083	-0.8858
C	2.7988	-1.2995	0.0000	C	-4.6724	-2.0603	0.0000	H	-4.2252	3.2320	0.0000
C	1.6538	-0.4969	0.0000	C	-3.5523	-2.8459	0.0000	H	-6.4677	2.1844	0.0000
C	1.7834	0.9172	0.0000	C	-2.2701	-2.2592	0.0000	H	-6.6955	-0.2934	0.0000
C	0.5979	1.7150	0.0000	C	-2.1126	-0.8894	0.0000	H	-5.6731	-2.5069	0.0000
C	0.3454	-1.0675	0.0000	H	7.3932	-1.5519	0.0000	H	-3.6364	-3.9376	0.0000
C	-0.7795	-0.2840	0.0000	H	7.6186	0.9125	0.0000	H	-1.3807	-2.9080	0.0000
C	-0.6444	1.1441	0.0000	H	5.6008	2.3650	-0.0000				

Table 3.259: Table of thermodynamic data as a function of temperature for 7*H*-Benzo[*de*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-48.208	406.327	406.327	∞
100	106.207	350.627	765.669	-41.504	433.342	481.241	-251.369
200	207.502	453.609	583.955	-26.069	419.075	534.822	-139.678
250	266.552	506.203	563.121	-14.229	412.346	564.538	-117.951
298.15	324.392	558.106	558.106	0.000	406.327	594.410	-104.136
300	326.592	560.119	558.112	0.602	406.105	595.576	-103.697
350	384.563	614.859	562.303	18.395	400.531	627.607	-93.663
400	438.499	669.783	572.306	38.991	395.670	660.379	-86.235
450	487.491	724.309	586.172	62.162	391.454	693.725	-80.524
500	531.389	777.988	602.678	87.655	387.800	727.530	-76.003
600	605.257	881.663	640.612	144.631	381.895	796.062	-69.302
700	663.953	979.540	682.111	208.201	377.636	865.454	-64.580
800	711.243	1071.395	725.092	277.043	374.828	935.339	-61.070
900	749.935	1157.475	768.404	350.164	373.283	1005.495	-58.356
1000	782.003	1238.200	811.390	426.809	372.821	1075.775	-56.192
1100	808.850	1314.028	853.673	506.391	373.241	1146.065	-54.421
1200	831.507	1385.406	895.040	588.440	374.391	1216.267	-52.942
1300	850.757	1452.743	935.375	672.579	376.087	1286.361	-51.686
1400	867.210	1516.409	974.624	758.498	378.194	1356.312	-50.604
1500	881.350	1576.734	1012.772	845.944	380.626	1426.101	-49.660
1600	893.565	1634.015	1049.825	934.704	383.253	1495.713	-48.829
1700	904.169	1688.512	1085.805	1024.603	386.000	1565.133	-48.090
1800	913.418	1740.461	1120.743	1115.493	388.793	1634.450	-47.430
1900	921.522	1790.069	1154.675	1207.248	391.597	1703.563	-46.833
2000	928.654	1837.522	1187.639	1299.765	394.359	1772.553	-46.293
2100	934.956	1882.986	1219.676	1392.952	397.002	1841.394	-45.801
2200	940.547	1926.612	1250.825	1486.732	399.526	1910.116	-45.351
2300	945.527	1968.533	1281.124	1581.041	401.921	1978.723	-44.937
2400	949.978	2008.870	1310.612	1675.820	404.123	2047.186	-44.555
2500	953.970	2047.733	1339.324	1771.021	406.139	2115.667	-44.204
2600	957.562	2085.219	1367.296	1866.601	407.934	2183.963	-43.875
2700	960.805	2121.420	1394.560	1962.522	409.513	2252.259	-43.572
2800	963.741	2156.416	1421.148	2058.751	410.851	2320.524	-43.289
2900	966.407	2190.282	1447.089	2155.261	411.919	2388.695	-43.024
3000	968.834	2223.086	1472.411	2252.025	412.756	2456.857	-42.777
3100	971.049	2254.891	1497.142	2349.020	413.292	2524.926	-42.544
3200	973.076	2285.753	1521.306	2446.228	413.564	2593.050	-42.326
3300	974.935	2315.725	1544.928	2543.630	413.554	2661.204	-42.122
3400	976.644	2344.855	1568.029	2641.210	413.237	2729.286	-41.930
3500	978.218	2373.189	1590.630	2738.954	412.616	2797.363	-41.747
3600	979.671	2400.767	1612.753	2836.850	411.711	2865.541	-41.577
3700	981.014	2427.627	1634.415	2934.885	410.495	2933.768	-41.417
3800	982.260	2453.806	1655.635	3033.049	408.939	3001.972	-41.264
3900	983.415	2479.336	1676.430	3131.334	407.084	3070.178	-41.120
4000	984.490	2504.247	1696.815	3229.729	404.914	3138.561	-40.985
4100	985.490	2528.569	1716.806	3328.229	402.396	3206.934	-40.856
4200	986.424	2552.329	1736.418	3426.825	399.555	3275.364	-40.734
4300	987.296	2575.550	1755.663	3525.512	396.378	3343.783	-40.618
4400	988.111	2598.257	1774.556	3624.283	392.873	3412.365	-40.509
4500	988.876	2620.471	1793.108	3723.132	389.054	3481.085	-40.407
4600	989.592	2642.213	1811.332	3822.056	384.873	3549.896	-40.310
4700	990.266	2663.503	1829.237	3921.049	380.342	3618.698	-40.216
4800	990.899	2684.358	1846.836	4020.108	375.507	3687.697	-40.129
4900	991.495	2704.796	1864.137	4119.228	370.297	3756.676	-40.046
5000	992.057	2724.833	1881.152	4218.406	364.800	3825.941	-39.969

3.260. Rubicene



Other names: Diindeno[1,2,3-*de*,1',2',3'-*kl*]anthracene

Formula: C₂₆H₁₄

Mass: 326.389 g/mol

CAS Number: 197-61-5

Point Group: C_{2h}

Length: 14.75 Å

Width: 10.76 Å

Breadth: 3.891 Å

L/B Ratio: 1.371

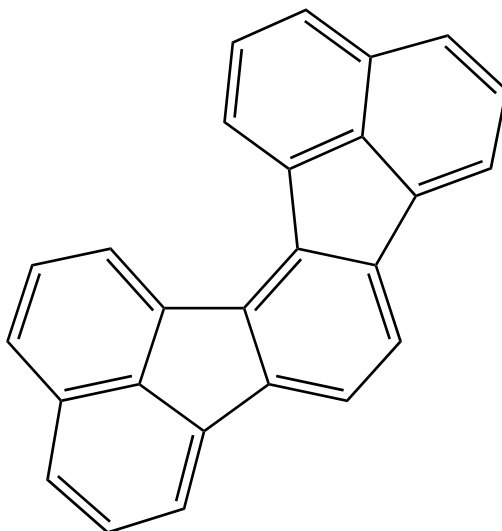
Cartesian coordinates:

C	4.7089	0.8221	0.0000	C	-1.0268	-0.8568	0.0000	H	-5.1576	-1.8204	0.0000
C	3.3385	0.6611	0.0000	C	-1.3130	0.5282	0.0000	H	-3.1027	2.7740	0.0000
C	2.7704	-0.6520	0.0000	C	0.3083	-2.8693	0.0000	H	-3.0375	-3.6326	0.0000
C	3.5697	-1.7774	0.0000	C	-0.8473	-3.5985	0.0000	H	-0.7979	-4.6930	0.0000
C	4.9575	-1.5981	0.0000	C	-2.1477	-2.9952	0.0000	H	1.3057	-3.3380	0.0000
C	5.5129	-0.3255	0.0000	C	-2.2392	-1.6376	0.0000	H	3.0375	3.6326	0.0000
C	2.2392	1.6377	0.0000	C	-3.3385	-0.6611	0.0000	H	0.7978	4.6929	0.0000
C	2.1477	2.9952	0.0000	C	-4.7089	-0.8221	0.0000	H	-1.3057	3.3380	0.0000
C	0.8472	3.5985	0.0000	C	-5.5130	0.3255	0.0000	H	3.1026	-2.7739	0.0000
C	-0.3083	2.8693	0.0000	C	-4.9575	1.5982	0.0000	H	5.6116	-2.4762	0.0000
C	-0.2543	1.4393	0.0000	C	-3.5697	1.7774	0.0000	H	6.6022	-0.2120	0.0000
C	1.0268	0.8568	0.0000	C	-2.7704	0.6520	0.0000	H	5.1576	1.8204	0.0000
C	1.3131	-0.5282	0.0000	H	-5.6115	2.4763	0.0000				
C	0.2544	-1.4393	0.0000	H	-6.6022	0.2120	0.0000				

Table 3.260: Table of thermodynamic data as a function of temperature for Rubicene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-47.643	504.267	504.267	∞
100	105.696	337.929	749.096	-41.117	527.192	566.383	-295.842
200	205.370	440.094	569.141	-25.810	515.165	610.350	-159.404
250	263.875	492.149	548.513	-14.091	509.416	634.810	-132.633
298.15	321.330	543.546	543.546	0.000	504.267	659.440	-115.529
300	323.516	545.541	543.552	0.596	504.076	660.401	-114.984
350	381.087	599.777	547.704	18.225	499.316	686.843	-102.504
400	434.572	654.208	557.617	38.636	495.176	713.913	-93.226
450	483.058	708.243	571.357	61.599	491.584	741.475	-86.066
500	526.400	761.426	587.713	86.856	488.459	769.432	-80.380
600	599.026	864.084	625.296	143.273	483.345	826.132	-71.920
700	656.350	960.899	666.396	206.152	479.560	883.586	-65.933
800	702.211	1051.646	708.943	274.162	476.953	941.486	-61.471
900	739.485	1136.579	751.792	346.309	475.372	999.643	-58.017
1000	770.200	1216.132	794.291	421.841	474.678	1057.940	-55.260
1100	795.792	1290.776	836.069	500.178	474.698	1116.280	-53.007
1200	817.306	1360.968	876.915	580.863	475.311	1174.573	-51.127
1300	835.529	1427.127	916.719	663.530	476.357	1232.808	-49.534
1400	851.066	1489.630	955.430	747.880	477.719	1290.953	-48.165
1500	864.393	1548.813	993.033	833.670	479.328	1348.994	-46.975
1600	875.886	1604.976	1029.540	920.697	481.069	1406.913	-45.930
1700	885.851	1658.382	1064.973	1008.796	482.878	1464.699	-45.004
1800	894.533	1709.267	1099.364	1097.825	484.687	1522.439	-44.179
1900	902.134	1757.840	1132.752	1187.667	486.470	1580.029	-43.437
2000	908.817	1804.287	1165.176	1278.221	488.181	1637.551	-42.768
2100	914.720	1848.774	1196.677	1369.404	489.748	1694.977	-42.159
2200	919.954	1891.450	1227.294	1461.143	491.172	1752.335	-41.605
2300	924.613	1932.448	1257.068	1553.376	492.449	1809.631	-41.097
2400	928.776	1971.889	1286.036	1646.049	493.516	1866.829	-40.630
2500	932.509	2009.881	1314.234	1739.117	494.383	1924.094	-40.201
2600	935.866	2046.521	1341.699	1832.538	495.019	1981.218	-39.802
2700	938.897	2081.899	1368.462	1926.279	495.428	2038.392	-39.434
2800	941.639	2116.094	1394.556	2020.308	495.586	2095.574	-39.093
2900	944.129	2149.182	1420.010	2114.598	495.466	2152.706	-38.774
3000	946.396	2181.228	1444.853	2209.126	495.111	2209.871	-38.476
3100	948.464	2212.295	1469.110	2303.871	494.448	2266.979	-38.198
3200	950.357	2242.437	1492.808	2398.813	493.516	2324.184	-37.938
3300	952.092	2271.708	1515.970	2493.937	492.300	2381.459	-37.695
3400	953.687	2300.155	1538.618	2589.227	490.772	2438.692	-37.465
3500	955.156	2327.822	1560.773	2684.670	488.938	2495.958	-37.249
3600	956.512	2354.749	1582.456	2780.254	486.819	2553.365	-37.048
3700	957.765	2380.973	1603.684	2875.969	484.386	2610.849	-36.858
3800	958.927	2406.531	1624.477	2971.804	481.614	2668.348	-36.678
3900	960.005	2431.454	1644.851	3067.752	478.543	2725.872	-36.508
4000	961.008	2455.772	1664.821	3163.803	475.156	2783.613	-36.350
4100	961.941	2479.513	1684.403	3259.951	471.421	2841.373	-36.199
4200	962.812	2502.704	1703.611	3356.189	467.364	2899.219	-36.056
4300	963.625	2525.369	1722.459	3452.511	462.972	2957.079	-35.921
4400	964.386	2547.531	1740.960	3548.912	458.254	3015.133	-35.793
4500	965.098	2569.212	1759.126	3645.387	453.224	3073.350	-35.674
4600	965.767	2590.431	1776.968	3741.930	447.831	3131.693	-35.561
4700	966.395	2611.208	1794.497	3838.539	442.092	3190.047	-35.453
4800	966.985	2631.560	1811.725	3935.208	436.048	3248.628	-35.352
4900	967.541	2651.504	1828.660	4031.935	429.631	3307.209	-35.255
5000	968.065	2671.056	1845.313	4128.715	422.928	3366.101	-35.165

3.261. Acenaphtho[1,2-*j*]fluoranthene



Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 193-21-5
Point Group: C_{2v}

Length: 15.11 Å
Width: 10.02 Å
Breadth: 3.884 Å
L/B Ratio: 1.509

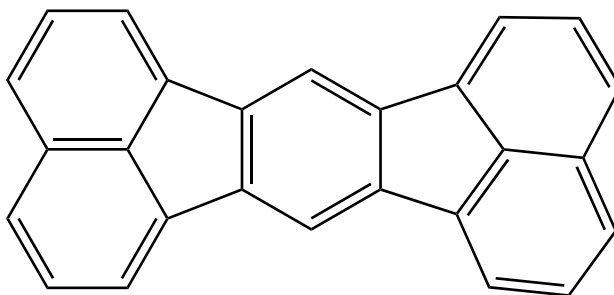
Cartesian coordinates:

C	4.2169	0.7931	0.0000	C	-0.7020	-2.6947	0.0000	H	-3.8536	-3.1438	0.0000
C	4.1977	2.2156	0.0000	C	0.7038	-2.6942	0.0000	H	-0.8269	2.8092	0.0000
C	2.9962	2.8797	0.0000	C	-1.7183	0.8395	0.0000	H	-2.9899	3.9734	0.0000
C	1.7413	2.2086	0.0000	C	-1.7428	2.2074	0.0000	H	-5.1479	2.7596	0.0000
C	1.7177	0.8406	0.0000	C	-2.9980	2.8777	0.0000	H	-1.2569	-3.6386	0.0000
C	2.9789	0.1623	0.0000	C	-4.1991	2.2128	0.0000	H	1.2595	-3.6377	0.0000
C	5.3594	-0.0551	0.0000	C	-4.2174	0.7904	0.0000	H	5.1462	2.7629	0.0000
C	5.2054	-1.4208	0.0000	C	-2.9791	0.1603	0.0000	H	2.9872	3.9754	0.0000
C	3.9297	-2.0492	0.0000	C	-2.8158	-1.2563	0.0000	H	0.8254	2.8103	0.0000
C	2.8166	-1.2543	0.0000	C	-3.9283	-2.0518	0.0000	H	3.8553	-3.1412	0.0000
C	1.3696	-1.4910	0.0000	C	-5.2045	-1.4242	0.0000	H	6.0930	-2.0631	0.0000
C	0.6882	-0.2146	0.0000	C	-5.3594	-0.0587	0.0000	H	6.3565	0.3978	0.0000
C	-0.6880	-0.2151	0.0000	H	-6.3568	0.3937	0.0000				
C	-1.3685	-1.4920	0.0000	H	-6.0916	-2.0671	0.0000				

Table 3.261: Table of thermodynamic data as a function of temperature for Acenaphtho[1,2-*j*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-47.236	502.286	502.286	∞
100	103.273	339.165	746.958	-40.779	525.549	564.617	-294.919
200	203.663	439.702	568.215	-25.703	513.292	608.555	-158.935
250	262.835	491.452	547.659	-14.052	507.474	633.042	-132.264
298.15	320.708	542.705	542.705	0.000	502.286	657.710	-115.226
300	322.906	544.695	542.711	0.595	502.095	658.673	-114.683
350	380.722	598.858	546.856	18.200	497.311	685.159	-102.252
400	434.339	653.249	556.757	38.597	493.156	712.276	-93.012
450	482.894	707.262	570.485	61.550	489.554	739.887	-85.882
500	526.271	760.429	586.830	86.800	486.422	767.893	-80.220
600	598.926	863.067	624.392	143.205	481.297	824.694	-71.795
700	656.261	959.868	665.475	206.075	477.502	882.251	-65.833
800	702.127	1050.603	708.007	274.076	474.887	940.254	-61.391
900	739.407	1135.527	750.844	346.215	473.297	998.516	-57.951
1000	770.127	1215.072	793.332	421.740	472.596	1056.918	-55.207
1100	795.725	1289.709	835.100	500.070	472.609	1115.364	-52.963
1200	817.245	1359.895	875.938	580.749	473.216	1173.765	-51.092
1300	835.473	1426.049	915.734	663.410	474.256	1232.107	-49.506
1400	851.015	1488.548	954.438	747.754	475.612	1290.360	-48.143
1500	864.345	1547.728	992.036	833.539	477.217	1348.509	-46.958
1600	875.842	1603.888	1028.537	920.562	478.953	1406.537	-45.918
1700	885.810	1657.292	1063.964	1008.656	480.758	1464.432	-44.996
1800	894.496	1708.175	1098.352	1097.681	482.563	1522.281	-44.175
1900	902.099	1756.746	1131.736	1187.520	484.343	1579.980	-43.436
2000	908.786	1803.191	1164.156	1278.071	486.050	1637.612	-42.769
2100	914.691	1847.677	1195.653	1369.251	487.614	1695.148	-42.164
2200	919.927	1890.351	1226.267	1460.987	489.035	1752.615	-41.612
2300	924.588	1931.349	1256.037	1553.217	490.310	1810.021	-41.106
2400	928.752	1970.788	1285.002	1645.888	491.374	1867.329	-40.641
2500	932.486	2008.779	1313.198	1738.953	492.239	1924.705	-40.214
2600	935.846	2045.418	1340.660	1832.372	492.873	1981.939	-39.817
2700	938.877	2080.795	1367.421	1926.111	493.279	2039.223	-39.450
2800	941.621	2114.990	1393.512	2020.138	493.436	2096.516	-39.110
2900	944.112	2148.077	1418.964	2114.427	493.314	2153.758	-38.793
3000	946.380	2180.123	1443.805	2208.953	492.958	2211.034	-38.497
3100	948.449	2211.189	1468.061	2303.696	492.293	2268.252	-38.219
3200	950.342	2241.331	1491.757	2398.637	491.359	2325.567	-37.960
3300	952.078	2270.602	1514.917	2493.759	490.142	2382.954	-37.718
3400	953.674	2299.048	1537.563	2589.048	488.612	2440.297	-37.490
3500	955.144	2326.714	1559.717	2684.490	486.777	2497.674	-37.275
3600	956.500	2353.641	1581.398	2780.073	484.657	2555.191	-37.074
3700	957.754	2379.865	1602.625	2875.787	482.223	2612.786	-36.885
3800	958.917	2405.422	1623.417	2971.621	479.450	2670.396	-36.706
3900	959.995	2430.345	1643.789	3067.567	476.377	2728.031	-36.537
4000	960.998	2454.663	1663.758	3163.617	472.990	2785.883	-36.379
4100	961.932	2478.404	1683.339	3259.764	469.254	2843.753	-36.229
4200	962.803	2501.595	1702.547	3356.002	465.196	2901.710	-36.087
4300	963.617	2524.259	1721.394	3452.323	460.803	2959.682	-35.952
4400	964.378	2546.421	1739.893	3548.723	456.085	3017.847	-35.826
4500	965.091	2568.102	1758.058	3645.197	451.053	3076.175	-35.707
4600	965.759	2589.321	1775.899	3741.740	445.660	3134.628	-35.594
4700	966.388	2610.097	1793.428	3838.348	439.920	3193.094	-35.487
4800	966.978	2630.449	1810.654	3935.016	433.875	3251.786	-35.386
4900	967.534	2650.394	1827.589	4031.742	427.457	3310.478	-35.289
5000	968.059	2669.946	1844.241	4128.522	420.754	3369.481	-35.200

3.262. Acenaphtho[1,2-*k*]fluoranthene



Other names: Benzo[1,2-*a*,4,5-*a'*]diacenaphthylene
3,4,1,6-Di(1,8-naphthylene)benzene

Formula: C₂₆H₁₄

Mass: 326.389 g/mol

CAS Number: 207-02-3

Point Group: D_{2h}

Length: 15.38 Å

Width: 9.208 Å

Breadth: 3.884 Å

L/B Ratio: 1.670

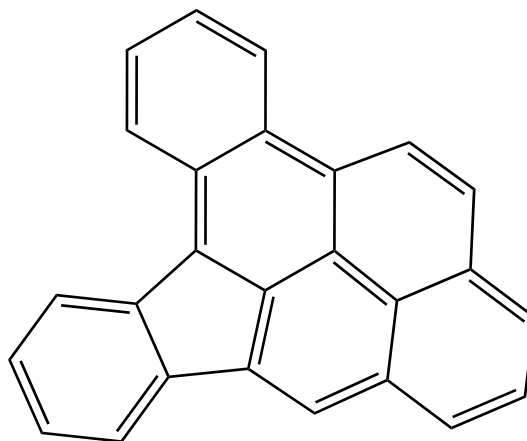
Cartesian coordinates:

C	4.7680	0.0016	0.0000	C	0.0006	-1.4420	0.0000	H	-2.6386	-3.3359	0.0000
C	5.3923	1.2809	0.0000	C	1.1831	-0.7140	0.0000	H	-2.6412	3.3339	0.0000
C	4.6256	2.4218	0.0000	C	-2.5763	1.1806	0.0000	H	-5.1213	3.3965	0.0000
C	3.2024	2.3977	0.0000	C	-3.2041	2.3953	0.0000	H	-6.4868	1.3343	0.0000
C	2.5754	1.1826	0.0000	C	-4.6273	2.4185	0.0000	H	0.0011	-2.5365	0.0000
C	3.3798	0.0014	0.0000	C	-5.3931	1.2770	0.0000	H	-0.0004	2.5367	0.0000
C	5.3928	-1.2774	0.0000	C	-4.7680	-0.0018	0.0000	H	6.4859	1.3389	0.0000
C	4.6268	-2.4188	0.0000	C	-3.3797	-0.0012	0.0000	H	5.1189	3.4002	0.0000
C	3.2035	-2.3952	0.0000	C	-2.5754	-1.1824	0.0000	H	2.6390	3.3359	0.0000
C	2.5763	-1.1803	0.0000	C	-3.2020	-2.3977	0.0000	H	2.6408	-3.3338	0.0000
C	1.1826	0.7153	0.0000	C	-4.6253	-2.4221	0.0000	H	5.1205	-3.3969	0.0000
C	-0.0006	1.4423	0.0000	C	-5.3921	-1.2813	0.0000	H	6.4864	-1.3348	0.0000
C	-1.1831	0.7143	0.0000	H	-6.4857	-1.3393	0.0000				
C	-1.1826	-0.7151	0.0000	H	-5.1183	-3.4006	0.0000				

Table 3.262: Table of thermodynamic data as a function of temperature for Acenaphtho[1,2-*k*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-47.158	487.613	487.613	∞
100	103.133	331.120	738.847	-40.773	510.883	550.755	-287.679
200	203.613	431.570	560.110	-25.708	498.613	595.503	-155.526
250	262.898	483.321	539.549	-14.057	492.796	620.397	-129.622
298.15	320.847	534.592	534.592	0.000	487.613	645.456	-113.079
300	323.047	536.584	534.598	0.596	487.422	646.434	-112.552
350	380.898	590.771	538.746	18.209	482.646	673.325	-100.486
400	434.523	645.187	548.651	38.614	478.501	700.846	-91.519
450	483.074	699.221	562.385	61.576	474.907	728.859	-84.602
500	526.446	752.407	578.737	86.835	471.785	757.267	-79.109
600	599.102	855.077	616.313	143.258	466.676	814.869	-70.939
700	656.455	951.905	657.411	206.146	462.900	873.223	-65.159
800	702.347	1042.668	699.958	274.168	460.306	932.021	-60.853
900	739.650	1127.620	742.808	346.330	458.739	991.075	-57.519
1000	770.389	1207.191	785.311	421.880	458.063	1050.267	-54.859
1100	795.996	1281.854	827.093	500.237	458.104	1109.500	-52.685
1200	817.519	1352.064	867.944	580.943	458.738	1168.684	-50.870
1300	835.745	1418.240	907.754	663.631	459.805	1227.809	-49.333
1400	851.281	1480.759	946.471	748.003	461.188	1286.841	-48.012
1500	864.603	1539.957	984.081	833.814	462.819	1345.769	-46.863
1600	876.090	1596.133	1020.594	920.862	464.581	1404.573	-45.854
1700	886.047	1649.551	1056.033	1008.981	466.409	1463.243	-44.959
1800	894.720	1700.447	1090.431	1098.029	468.237	1521.865	-44.162
1900	902.312	1749.030	1123.826	1187.889	470.039	1580.336	-43.446
2000	908.987	1795.486	1156.256	1278.461	471.767	1638.739	-42.799
2100	914.881	1839.981	1187.762	1369.660	473.351	1697.045	-42.211
2200	920.106	1882.665	1218.385	1461.415	474.790	1755.281	-41.675
2300	924.757	1923.670	1248.164	1553.663	476.083	1813.456	-41.184
2400	928.913	1963.116	1277.137	1646.350	477.163	1871.531	-40.732
2500	932.638	2001.113	1305.341	1739.431	478.044	1929.673	-40.317
2600	935.989	2037.758	1332.810	1832.865	478.692	1987.674	-39.932
2700	939.012	2073.141	1359.579	1926.618	479.113	2045.724	-39.576
2800	941.749	2107.341	1385.677	2020.658	479.282	2103.782	-39.246
2900	944.234	2140.432	1411.136	2114.959	479.173	2161.789	-38.937
3000	946.495	2172.482	1435.982	2209.497	478.829	2219.829	-38.650
3100	948.558	2203.551	1460.244	2304.251	478.175	2277.811	-38.380
3200	950.446	2233.697	1483.946	2399.203	477.252	2335.890	-38.129
3300	952.177	2262.970	1507.111	2494.335	476.045	2394.039	-37.894
3400	953.768	2291.420	1529.763	2589.634	474.525	2452.146	-37.672
3500	955.233	2319.089	1551.921	2685.085	472.699	2510.285	-37.463
3600	956.585	2346.017	1573.607	2780.676	470.588	2568.565	-37.268
3700	957.836	2372.244	1594.839	2876.398	468.162	2626.922	-37.085
3800	958.994	2397.804	1615.635	2972.241	465.397	2685.294	-36.911
3900	960.069	2422.728	1636.011	3068.194	462.332	2743.691	-36.747
4000	961.069	2447.048	1655.985	3164.252	458.951	2802.305	-36.594
4100	962.000	2470.790	1675.570	3260.406	455.222	2860.936	-36.448
4200	962.868	2493.983	1694.781	3356.650	451.171	2919.655	-36.310
4300	963.679	2516.649	1713.631	3452.978	446.785	2978.387	-36.179
4400	964.437	2538.813	1732.134	3549.384	442.072	3037.313	-36.057
4500	965.148	2560.494	1750.302	3645.863	437.047	3096.402	-35.941
4600	965.815	2581.714	1768.147	3742.412	431.659	3155.616	-35.832
4700	966.441	2602.492	1785.678	3839.025	425.924	3214.842	-35.728
4800	967.029	2622.845	1802.908	3935.699	419.885	3274.295	-35.631
4900	967.584	2642.791	1819.846	4032.430	413.472	3333.747	-35.537
5000	968.106	2662.344	1836.501	4129.214	406.774	3393.510	-35.451

3.263. Fluoreno[3,2,1,9-*defg*]chrysene



Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 192-35-8
Point Group: C_s

Length: 13.75 Å
Width: 12.11 Å
Breadth: 3.887 Å
L/B Ratio: 1.135

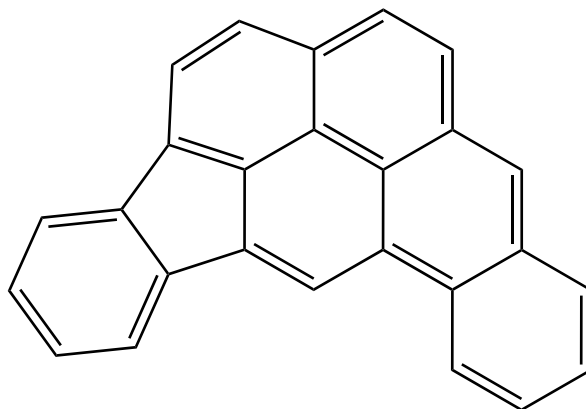
Cartesian coordinates:

C	4.6729	0.4980	0.0000	C	-2.7441	-3.6792	0.0000	H	3.4059	3.6661	0.0000
C	4.6252	1.8806	0.0000	C	-1.5412	-4.4202	0.0000	H	2.2611	-3.4821	0.0000
C	3.4069	2.5701	0.0000	C	-0.3324	-3.7770	0.0000	H	4.4111	-2.2124	0.0000
C	3.4795	-0.2458	0.0000	C	-0.1556	0.3983	0.0000	H	0.9194	3.6653	0.0000
C	2.2811	-2.3815	0.0000	C	-0.2240	1.8502	0.0000	H	-3.6404	-1.7158	0.0000
C	3.4508	-1.6838	0.0000	C	-1.4061	-0.2005	0.0000	H	-3.6999	-4.2132	0.0000
C	1.0179	-1.7042	0.0000	C	-2.3811	0.8992	0.0000	H	-1.5878	-5.5140	0.0000
C	2.2573	0.4523	0.0000	C	-1.6652	2.1423	0.0000	H	0.6165	-4.3361	0.0000
C	2.2024	1.8746	0.0000	C	-2.3471	3.3414	0.0000	H	-1.8075	4.2936	0.0000
C	0.9201	2.5698	0.0000	C	-3.7475	3.3113	0.0000	H	-4.3016	4.2558	0.0000
C	1.0523	-0.3086	0.0000	C	-4.4402	2.1089	0.0000	H	-5.5352	2.1133	0.0000
C	-0.2596	-2.3594	0.0000	C	-3.7615	0.8851	0.0000	H	-4.3002	-0.0736	0.0000
C	-1.4746	-1.6173	0.0000	H	5.6358	-0.0248	0.0000				
C	-2.7129	-2.3103	0.0000	H	5.5588	2.4537	0.0000				

Table 3.263: Table of thermodynamic data as a function of temperature for Fluoreno[3,2,1,9-*defg*]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-46.877	449.294	449.294	∞
100	101.609	337.556	744.023	-40.647	472.689	511.918	-267.393
200	203.276	437.512	565.742	-25.646	460.356	556.057	-145.224
250	262.263	489.160	545.233	-14.018	454.515	580.657	-121.319
298.15	319.894	540.291	540.291	0.000	449.294	605.438	-106.068
300	322.083	542.276	540.297	0.594	449.101	606.405	-105.582
350	379.710	596.297	544.432	18.153	444.271	633.015	-94.470
400	433.224	650.546	554.306	38.496	440.063	660.264	-86.220
450	481.745	704.424	567.999	61.391	436.403	688.014	-79.861
500	525.139	757.471	584.302	86.585	433.214	716.164	-74.816
600	597.899	859.911	621.775	142.881	427.980	773.272	-67.318
700	655.372	956.563	662.770	205.655	424.090	831.152	-62.020
800	701.371	1047.189	705.221	273.575	421.392	889.491	-58.077
900	738.766	1132.031	747.982	345.644	419.733	948.099	-55.025
1000	769.583	1211.513	790.404	421.109	418.973	1006.854	-52.592
1100	795.260	1286.102	832.112	499.389	418.936	1065.659	-50.603
1200	816.845	1356.251	872.897	580.025	419.500	1124.422	-48.944
1300	835.126	1422.375	912.646	662.648	420.502	1183.130	-47.538
1400	850.712	1484.850	951.307	746.960	421.826	1241.752	-46.329
1500	864.079	1544.011	988.866	832.717	423.403	1300.272	-45.279
1600	875.607	1600.154	1025.332	919.715	425.114	1358.672	-44.355
1700	885.602	1653.544	1060.728	1007.787	426.896	1416.942	-43.536
1800	894.309	1704.416	1095.087	1096.793	428.681	1475.165	-42.807
1900	901.931	1752.978	1128.444	1186.613	430.444	1533.241	-42.151
2000	908.634	1799.415	1160.840	1277.148	432.135	1591.250	-41.558
2100	914.552	1843.893	1192.315	1368.313	433.684	1649.164	-41.020
2200	919.801	1886.562	1222.909	1460.036	435.092	1707.010	-40.529
2300	924.472	1927.553	1252.660	1552.254	436.355	1764.795	-40.079
2400	928.646	1966.988	1281.608	1644.914	437.408	1822.483	-39.664
2500	932.389	2004.975	1309.787	1737.969	438.263	1880.239	-39.285
2600	935.755	2041.611	1337.234	1831.379	438.887	1937.853	-38.931
2700	938.793	2076.984	1363.981	1925.109	439.285	1995.519	-38.605
2800	941.543	2111.176	1390.059	2019.129	439.433	2053.193	-38.302
2900	944.040	2144.261	1415.499	2113.410	439.305	2110.816	-38.019
3000	946.312	2176.304	1440.328	2207.929	438.941	2168.474	-37.756
3100	948.385	2207.368	1464.572	2302.665	438.269	2226.074	-37.508
3200	950.283	2237.508	1488.258	2397.600	437.330	2283.771	-37.278
3300	952.022	2266.777	1511.408	2492.717	436.107	2341.540	-37.063
3400	953.621	2295.222	1534.045	2588.000	434.572	2399.266	-36.859
3500	955.094	2322.886	1556.190	2683.437	432.732	2457.026	-36.668
3600	956.453	2349.811	1577.863	2779.015	430.607	2514.926	-36.490
3700	957.710	2376.035	1599.082	2874.724	428.168	2572.904	-36.322
3800	958.874	2401.591	1619.866	2970.554	425.391	2630.897	-36.163
3900	959.955	2426.512	1640.231	3066.496	422.314	2688.915	-36.013
4000	960.960	2450.829	1660.193	3162.542	418.922	2747.151	-35.873
4100	961.896	2474.569	1679.768	3258.686	415.183	2805.404	-35.741
4200	962.768	2497.759	1698.969	3354.919	411.121	2863.745	-35.615
4300	963.584	2520.423	1717.810	3451.237	406.725	2922.100	-35.496
4400	964.346	2542.584	1736.304	3547.634	402.003	2980.648	-35.384
4500	965.061	2564.264	1754.463	3644.105	396.969	3039.360	-35.279
4600	965.731	2585.482	1772.299	3740.645	391.573	3098.197	-35.180
4700	966.360	2606.258	1789.822	3837.250	385.830	3157.047	-35.086
4800	966.952	2626.610	1807.044	3933.916	379.783	3216.123	-34.998
4900	967.509	2646.553	1823.974	4030.639	373.362	3275.198	-34.913
5000	968.034	2666.105	1840.622	4127.416	366.656	3334.586	-34.835

3.264. Benz[def]indeno[1,2,3-qr]chrysene



Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 111189-34-5
Point Group: C_s

Length: 14.99 Å
Width: 11.13 Å
Breadth: 3.885 Å
L/B Ratio: 1.347

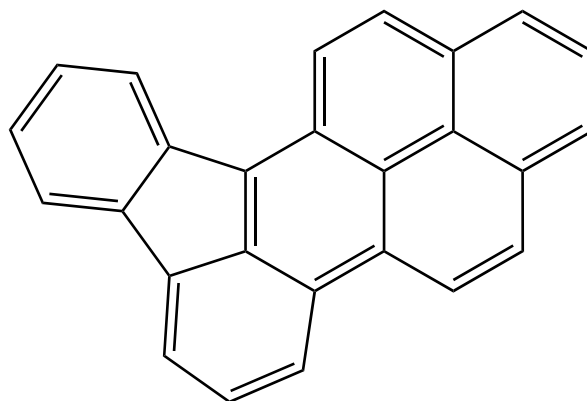
Cartesian coordinates:

C	5.3395	1.6229	0.0000	C	0.1848	-1.4239	0.0000	H	2.4571	3.4636	0.0000
C	4.5044	2.7301	0.0000	C	-1.1056	-0.8173	0.0000	H	5.4819	-0.5475	0.0000
C	3.1109	2.5859	0.0000	C	-2.2406	-1.6838	0.0000	H	1.9078	-4.3668	0.0000
C	4.8181	0.3228	0.0000	C	-2.0088	-3.1178	0.0000	H	3.8501	-2.8208	0.0000
C	3.4477	0.1657	0.0000	C	-0.7694	-3.6591	0.0000	H	-0.1910	2.5138	0.0000
C	2.5833	1.3116	0.0000	C	0.4113	-2.8221	0.0000	H	-4.3908	-1.7686	0.0000
C	2.6190	-1.0487	0.0000	C	-3.6617	0.2828	0.0000	H	-2.8956	-3.7628	0.0000
C	1.7258	-3.2860	0.0000	C	-2.5396	1.1412	0.0000	H	-0.6269	-4.7455	0.0000
C	2.8342	-2.4128	0.0000	C	-2.7489	2.5454	0.0000	H	-1.8633	3.1994	0.0000
C	1.2822	-0.5862	0.0000	C	-4.0153	3.0654	0.0000	H	-4.1716	4.1490	0.0000
C	1.1869	0.8497	0.0000	C	-5.1371	2.2066	0.0000	H	-6.1420	2.6415	0.0000
C	-0.0462	1.4230	0.0000	C	-4.9662	0.8483	0.0000	H	-5.8326	0.1770	0.0000
C	-1.2211	0.5813	0.0000	H	6.4256	1.7627	0.0000				
C	-3.4991	-1.1298	0.0000	H	4.9372	3.7360	0.0000				

Table 3.264: Table of thermodynamic data as a function of temperature for Benz[def]indeno[1,2,3-qr]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-47.035	445.885	445.885	∞
100	102.075	340.654	747.740	-40.709	469.218	508.137	-265.418
200	203.516	440.765	569.199	-25.687	456.906	551.956	-144.153
250	262.691	492.487	548.657	-14.042	451.082	576.392	-120.428
298.15	320.455	543.706	543.706	0.000	445.885	601.011	-105.292
300	322.648	545.695	543.712	0.595	445.693	601.972	-104.810
350	380.344	599.808	547.854	18.184	440.893	628.409	-93.783
400	433.877	654.143	557.745	38.559	436.717	655.480	-85.595
450	482.390	708.098	571.459	61.488	433.090	683.047	-79.284
500	525.760	761.212	587.787	86.712	429.933	711.013	-74.277
600	598.468	863.761	625.313	143.069	424.759	767.741	-66.836
700	655.895	960.497	666.359	205.897	420.923	825.231	-61.578
800	701.859	1051.190	708.856	273.867	418.276	883.173	-57.664
900	739.225	1136.087	751.662	345.983	416.664	941.378	-54.635
1000	770.016	1215.617	794.124	421.493	415.948	999.725	-52.219
1100	795.668	1290.246	835.869	499.815	415.953	1058.118	-50.245
1200	817.229	1360.429	876.687	580.491	416.557	1116.464	-48.597
1300	835.487	1426.583	916.467	663.151	417.596	1174.753	-47.201
1400	851.049	1489.084	955.157	747.498	418.955	1232.953	-46.001
1500	864.394	1548.267	992.742	833.287	420.564	1291.048	-44.957
1600	875.901	1604.430	1029.233	920.316	422.306	1349.022	-44.040
1700	885.876	1657.838	1064.652	1008.416	424.116	1406.863	-43.227
1800	894.565	1708.725	1099.031	1097.448	425.928	1464.657	-42.502
1900	902.170	1757.299	1132.408	1187.293	427.715	1522.301	-41.850
2000	908.856	1803.748	1164.823	1277.852	429.430	1579.877	-41.261
2100	914.760	1848.237	1196.314	1369.038	431.000	1637.357	-40.726
2200	919.995	1890.915	1226.924	1460.781	432.428	1694.768	-40.238
2300	924.655	1931.915	1256.690	1553.018	433.710	1752.118	-39.791
2400	928.817	1971.358	1285.651	1645.696	434.781	1809.369	-39.379
2500	932.549	2009.351	1313.844	1738.767	435.652	1866.687	-39.001
2600	935.906	2045.993	1341.303	1832.193	436.292	1923.864	-38.650
2700	938.935	2081.372	1368.062	1925.938	436.705	1981.091	-38.326
2800	941.677	2115.569	1394.151	2019.971	436.867	2038.326	-38.025
2900	944.166	2148.658	1419.601	2114.265	436.751	2095.510	-37.743
3000	946.431	2180.706	1444.440	2208.796	436.399	2152.727	-37.482
3100	948.498	2211.773	1468.694	2303.544	435.739	2209.888	-37.236
3200	950.389	2241.917	1492.389	2398.490	434.811	2267.144	-37.007
3300	952.123	2271.189	1515.547	2493.617	433.598	2324.472	-36.793
3400	953.717	2299.637	1538.193	2588.910	432.073	2381.756	-36.590
3500	955.185	2327.304	1560.345	2684.356	430.242	2439.074	-36.400
3600	956.540	2354.232	1582.025	2779.943	428.126	2496.533	-36.223
3700	957.793	2380.457	1603.252	2875.661	425.696	2554.068	-36.056
3800	958.953	2406.015	1624.042	2971.499	422.927	2611.619	-35.898
3900	960.030	2430.939	1644.414	3067.449	419.858	2669.195	-35.749
4000	961.032	2455.257	1664.382	3163.502	416.473	2726.987	-35.610
4100	961.964	2478.999	1683.962	3259.653	412.741	2784.798	-35.478
4200	962.834	2502.191	1703.169	3355.893	408.686	2842.695	-35.353
4300	963.647	2524.857	1722.015	3452.218	404.297	2900.607	-35.235
4400	964.407	2547.019	1740.514	3548.621	399.581	2958.712	-35.124
4500	965.118	2568.700	1758.679	3645.097	394.552	3016.980	-35.019
4600	965.786	2589.920	1776.519	3741.643	389.162	3075.374	-34.921
4700	966.413	2610.697	1794.047	3838.253	383.424	3133.779	-34.827
4800	967.003	2631.050	1811.274	3934.924	377.382	3192.411	-34.740
4900	967.558	2650.994	1828.208	4031.653	370.967	3251.043	-34.656
5000	968.082	2670.547	1844.860	4128.435	364.266	3309.986	-34.578

3.265. Benz[def]indeno[1,2,3-hi]chrysene



Formula: $C_{26}H_{14}$
Mass: 326.389 g/mol
CAS Number: 111189-33-4
Point Group: C_s

Length: 14.91 Å
Width: 10.79 Å
Breadth: 3.889 Å
L/B Ratio: 1.382

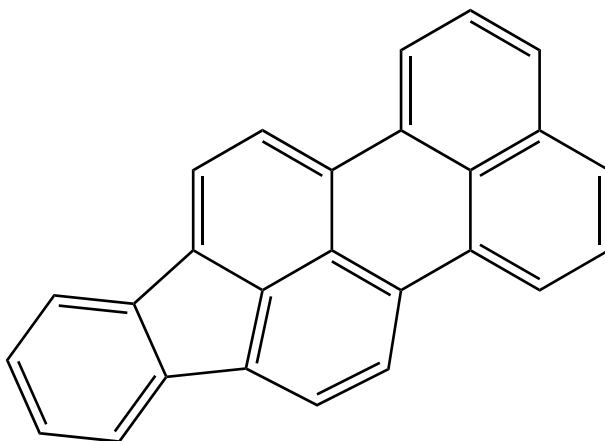
Cartesian coordinates:

C	4.2130	-2.6170	0.0000	C	-2.1512	2.3565	0.0000	H	5.5031	0.5512	0.0000
C	5.1522	-1.5954	0.0000	C	-3.4297	1.8997	0.0000	H	2.0934	-3.1422	0.0000
C	4.7588	-0.2514	0.0000	C	-3.7001	0.4929	0.0000	H	4.1229	2.9391	0.0000
C	2.8420	-2.3369	0.0000	C	-5.0207	0.0067	0.0000	H	2.3504	4.6797	0.0000
C	2.4389	-1.0159	0.0000	C	-5.2632	-1.3527	0.0000	H	-0.0701	4.0820	0.0000
C	3.4094	0.0367	0.0000	C	-4.2033	-2.2641	0.0000	H	-1.9186	3.4319	0.0000
C	2.7001	1.3220	0.0000	C	-0.1929	-0.8937	0.0000	H	-4.2772	2.5947	0.0000
C	3.0704	2.6390	0.0000	C	-1.2722	0.0640	0.0000	H	-5.8545	0.7181	0.0000
C	2.0479	3.6268	0.0000	C	-2.6224	-0.4188	0.0000	H	-6.2930	-1.7254	0.0000
C	0.7105	3.3082	0.0000	C	-2.8889	-1.8128	0.0000	H	-4.4120	-3.3401	0.0000
C	1.3079	0.9972	0.0000	C	-1.7805	-2.7410	0.0000	H	-2.0111	-3.8127	0.0000
C	0.2976	1.9480	0.0000	C	-0.5055	-2.3038	0.0000	H	0.3440	-3.0054	0.0000
C	1.0981	-0.4168	0.0000	H	4.5457	-3.6602	0.0000				
C	-1.0449	1.4511	0.0000	H	6.2196	-1.8399	0.0000				

Table 3.265: Table of thermodynamic data as a function of temperature for Benz[def]indeno[1,2,3-hi]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-46.918	442.391	442.391	∞
100	101.415	339.780	746.142	-40.636	465.797	504.803	-263.677
200	203.235	439.603	567.871	-25.654	453.446	548.728	-143.310
250	262.355	491.257	547.355	-14.025	447.607	573.223	-119.766
298.15	320.048	542.410	542.410	0.000	442.391	597.903	-104.748
300	322.239	544.397	542.417	0.594	442.198	598.867	-104.270
350	379.886	598.443	546.553	18.161	437.377	625.370	-93.329
400	433.401	652.716	556.432	38.513	433.178	652.511	-85.207
450	481.915	706.615	570.131	61.418	429.527	680.152	-78.948
500	525.298	759.679	586.441	86.619	426.346	708.192	-73.983
600	598.037	862.146	623.928	142.931	421.127	765.078	-66.605
700	655.491	958.818	664.936	205.717	417.250	822.733	-61.392
800	701.472	1049.458	707.399	273.648	414.563	880.846	-57.512
900	738.853	1134.311	750.171	345.726	412.913	939.226	-54.510
1000	769.658	1213.802	792.602	421.200	412.161	997.753	-52.116
1100	795.325	1288.398	834.319	499.487	412.131	1056.328	-50.160
1200	816.902	1358.552	875.112	580.129	412.701	1114.861	-48.528
1300	835.177	1424.681	914.867	662.758	413.709	1173.339	-47.144
1400	850.757	1487.159	953.535	747.075	415.038	1231.730	-45.955
1500	864.119	1546.323	991.099	832.835	416.619	1290.019	-44.922
1600	875.643	1602.469	1027.570	919.837	418.334	1348.188	-44.013
1700	885.634	1655.861	1062.971	1007.913	420.119	1406.226	-43.207
1800	894.338	1706.735	1097.334	1096.921	421.908	1464.218	-42.490
1900	901.958	1755.298	1130.695	1186.744	423.673	1522.062	-41.844
2000	908.658	1801.736	1163.095	1277.282	425.366	1579.839	-41.260
2100	914.575	1846.216	1194.573	1368.450	426.918	1637.521	-40.730
2200	919.821	1888.885	1225.169	1460.175	428.328	1695.134	-40.247
2300	924.491	1929.878	1254.923	1552.395	429.593	1752.687	-39.804
2400	928.664	1969.314	1283.873	1645.056	430.648	1810.142	-39.396
2500	932.405	2007.301	1312.055	1738.113	431.505	1867.665	-39.022
2600	935.770	2043.937	1339.504	1831.525	432.130	1925.048	-38.674
2700	938.807	2079.311	1366.253	1925.256	432.530	1982.480	-38.353
2800	941.556	2113.504	1392.334	2019.277	432.679	2039.921	-38.054
2900	944.052	2146.589	1417.775	2113.559	432.551	2097.312	-37.776
3000	946.323	2178.632	1442.606	2208.080	432.189	2154.737	-37.517
3100	948.396	2209.696	1466.852	2302.817	431.518	2212.105	-37.273
3200	950.293	2239.837	1490.539	2397.753	430.580	2269.569	-37.046
3300	952.032	2269.106	1513.691	2492.870	429.358	2327.105	-36.834
3400	953.630	2297.551	1536.329	2588.155	427.824	2384.598	-36.634
3500	955.102	2325.216	1558.475	2683.592	425.985	2442.124	-36.446
3600	956.461	2352.141	1580.149	2779.171	423.861	2499.792	-36.270
3700	957.717	2378.365	1601.370	2874.881	421.422	2557.537	-36.105
3800	958.882	2403.921	1622.155	2970.712	418.646	2615.296	-35.949
3900	959.962	2428.843	1642.521	3066.655	415.570	2673.082	-35.801
4000	960.966	2453.160	1662.484	3162.702	412.179	2731.084	-35.664
4100	961.902	2476.900	1682.060	3258.846	408.440	2789.105	-35.533
4200	962.774	2500.090	1701.262	3355.080	404.379	2847.212	-35.410
4300	963.589	2522.754	1720.104	3451.398	399.984	2905.334	-35.292
4400	964.352	2544.916	1738.598	3547.796	395.262	2963.650	-35.182
4500	965.066	2566.595	1756.758	3644.267	390.228	3022.128	-35.079
4600	965.736	2587.814	1774.595	3740.808	384.833	3080.732	-34.982
4700	966.365	2608.590	1792.119	3837.413	379.090	3139.348	-34.889
4800	966.956	2628.942	1809.342	3934.079	373.044	3198.191	-34.803
4900	967.513	2648.885	1826.272	4030.803	366.623	3257.034	-34.720
5000	968.038	2668.437	1842.921	4127.581	359.918	3316.188	-34.643

3.266. Indeno[1,2,3-*cd*]perylene



Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 101686-49-1
Point Group: C_{2v}

Length: 15.32 Å
Width: 9.178 Å
Breadth: 3.884 Å
L/B Ratio: 1.669

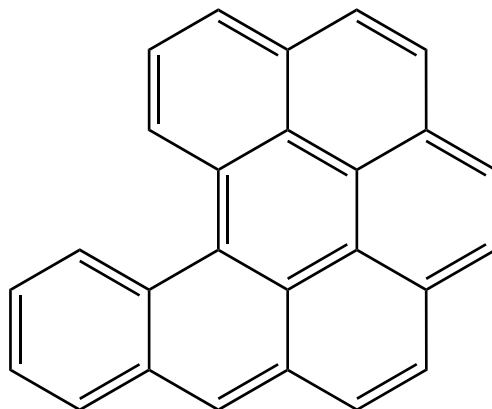
Cartesian coordinates:

C	5.9375	-0.4531	0.0000	C	-0.7452	1.2365	0.0000	H	4.6153	2.7014	0.0000
C	5.8813	0.9329	0.0000	C	-0.6424	-1.2928	0.0000	H	4.8187	-2.3183	0.0000
C	4.6540	1.6076	0.0000	C	-2.1009	-1.3416	0.0000	H	1.9112	3.4199	0.0000
C	4.7688	-1.2250	0.0000	C	-4.9046	-1.4339	0.0000	H	-0.5889	3.3665	0.0000
C	3.5529	-0.5735	0.0000	C	-4.1762	-2.5934	0.0000	H	-0.3144	-3.4029	0.0000
C	3.4947	0.8597	0.0000	C	-2.7678	-2.5479	0.0000	H	2.1827	-3.2534	0.0000
C	2.0843	1.2718	0.0000	C	-2.8399	-0.1153	0.0000	H	-6.0003	-1.4608	0.0000
C	1.3937	2.4555	0.0000	C	-2.2028	1.1668	0.0000	H	-4.6772	-3.5670	0.0000
C	-0.0268	2.4195	0.0000	C	-2.9654	2.3151	0.0000	H	-2.1817	-3.4801	0.0000
C	2.1805	-1.0986	0.0000	C	-4.3728	2.2462	0.0000	H	-2.4569	3.2919	0.0000
C	1.3390	0.0544	0.0000	C	-5.0048	1.0314	0.0000	H	-4.9512	3.1759	0.0000
C	0.1696	-2.4137	0.0000	C	-4.2501	-0.1726	0.0000	H	-6.0991	0.9694	0.0000
C	1.5881	-2.3344	0.0000	H	6.9101	-0.9562	0.0000				
C	-0.0428	-0.0017	0.0000	H	6.8100	1.5130	0.0000				

Table 3.266: Table of thermodynamic data as a function of temperature for Indeno[1,2,3-*cd*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-46.826	459.230	459.230	∞
100	101.553	334.310	739.580	-40.527	482.746	522.299	-272.815
200	202.576	433.932	561.822	-25.578	470.360	566.777	-148.024
250	261.565	485.423	541.365	-13.986	464.485	591.560	-123.597
298.15	319.238	536.434	536.434	0.000	459.230	616.524	-108.010
300	321.429	538.416	536.440	0.593	459.036	617.499	-107.514
350	379.124	592.340	540.567	18.120	454.175	644.304	-96.155
400	432.715	646.516	550.425	38.436	449.940	671.753	-87.720
450	481.314	700.339	564.098	61.308	446.257	699.705	-81.218
500	524.778	753.344	580.381	86.482	443.048	728.062	-76.059
600	597.656	855.729	617.815	142.749	437.784	785.585	-68.390
700	655.215	952.351	658.776	205.503	433.874	843.885	-62.970
800	701.275	1042.959	701.197	273.410	431.164	902.646	-58.936
900	738.713	1127.793	743.936	345.471	429.498	961.677	-55.813
1000	769.561	1207.271	786.338	420.933	428.734	1020.857	-53.323
1100	795.259	1281.860	828.030	499.212	428.696	1080.085	-51.288
1200	816.858	1352.009	868.802	579.849	429.260	1139.273	-49.590
1300	835.149	1418.134	908.539	662.474	430.264	1198.405	-48.152
1400	850.741	1480.611	947.191	746.789	431.591	1257.451	-46.915
1500	864.112	1539.774	984.742	832.548	433.171	1316.395	-45.840
1600	875.642	1595.920	1021.201	919.550	434.885	1375.219	-44.895
1700	885.637	1649.312	1056.591	1007.626	436.671	1433.911	-44.058
1800	894.345	1700.186	1090.944	1096.635	438.460	1492.558	-43.312
1900	901.967	1748.749	1124.297	1186.458	440.226	1551.057	-42.641
2000	908.668	1795.188	1156.690	1276.997	441.921	1609.488	-42.035
2100	914.586	1839.668	1188.161	1368.166	443.473	1667.825	-41.484
2200	919.833	1882.338	1218.751	1459.892	444.885	1726.093	-40.982
2300	924.504	1923.332	1248.500	1552.113	446.151	1784.301	-40.522
2400	928.676	1962.768	1277.445	1644.776	447.207	1842.411	-40.098
2500	932.417	2000.756	1305.622	1737.834	448.065	1900.588	-39.710
2600	935.783	2037.392	1333.067	1831.247	448.692	1958.625	-39.348
2700	938.819	2072.767	1359.812	1924.980	449.092	2016.712	-39.015
2800	941.568	2106.960	1385.888	2019.001	449.243	2074.808	-38.705
2900	944.063	2140.045	1411.326	2113.285	449.116	2132.853	-38.416
3000	946.334	2172.089	1436.154	2207.807	448.755	2190.932	-38.147
3100	948.407	2203.154	1460.397	2302.545	448.086	2248.954	-37.894
3200	950.303	2233.295	1484.082	2397.482	447.149	2307.072	-37.658
3300	952.042	2262.564	1507.231	2492.601	445.927	2365.262	-37.438
3400	953.640	2291.010	1529.867	2587.886	444.394	2423.410	-37.230
3500	955.112	2318.675	1552.011	2683.324	442.556	2481.590	-37.035
3600	956.470	2345.600	1573.682	2778.904	440.433	2539.912	-36.852
3700	957.726	2371.824	1594.901	2874.615	437.995	2598.311	-36.681
3800	958.890	2397.381	1615.684	2970.447	435.220	2656.725	-36.518
3900	959.970	2422.302	1636.048	3066.390	432.145	2715.164	-36.365
4000	960.974	2446.619	1656.010	3162.438	428.754	2773.821	-36.222
4100	961.909	2470.360	1675.584	3258.583	425.016	2832.495	-36.086
4200	962.782	2493.550	1694.784	3354.818	420.956	2891.256	-35.957
4300	963.596	2516.215	1713.625	3451.137	416.562	2950.033	-35.835
4400	964.358	2538.376	1732.118	3547.535	411.841	3009.002	-35.721
4500	965.072	2560.056	1750.277	3644.007	406.808	3068.134	-35.613
4600	965.742	2581.275	1768.112	3740.548	401.413	3127.392	-35.512
4700	966.371	2602.051	1785.635	3837.154	395.671	3186.662	-35.415
4800	966.962	2622.403	1802.857	3933.821	389.625	3246.159	-35.325
4900	967.519	2642.347	1819.786	4030.546	383.205	3305.656	-35.238
5000	968.044	2661.898	1836.434	4127.324	376.500	3365.464	-35.158

3.267. Dibenzo[*a,ghi*]perylene



Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 6596-37-8
Point Group: C₁

Length: 13.78 Å
Width: 11.62 Å
Breadth: 4.839 Å
L/B Ratio: 1.186

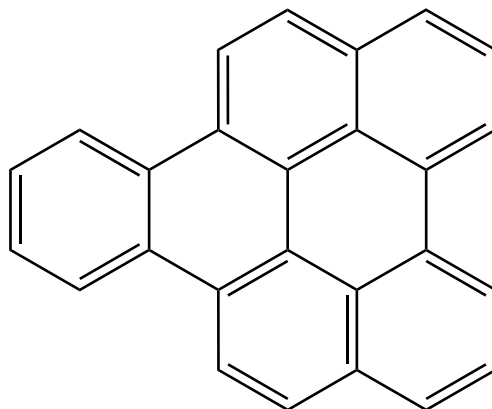
Cartesian coordinates:

C	4.4467	1.4179	-0.5847	C	0.3174	-1.0498	0.1220	H	5.0947	-1.8362	0.1847
C	5.1926	0.2453	-0.3144	C	-1.1144	-1.1811	0.0241	H	2.5322	2.3354	-0.7104
C	4.5392	-0.9096	-0.0009	C	0.0960	1.3977	0.1855	H	3.0634	-3.0833	0.4237
C	3.0858	1.4162	-0.4751	C	-1.5840	3.6768	0.2733	H	1.0454	-4.4174	0.4346
C	2.3618	0.2486	-0.0877	C	-0.2378	3.7824	0.5579	H	-1.4219	-4.5961	0.2177
C	3.1144	-0.9419	0.0769	C	0.5883	2.6575	0.5205	H	-3.5822	-3.5442	-0.1706
C	2.4660	-2.1747	0.2770	C	-1.3098	1.2712	0.0136	H	-4.9803	-1.5103	-0.4443
C	1.0869	-2.2448	0.2369	C	-1.9187	-0.0205	-0.0983	H	-2.2267	4.5642	0.2706
C	0.4232	-3.5246	0.3022	C	-3.3086	-0.1418	-0.2635	H	0.1949	4.7563	0.8111
C	-0.9183	-3.6232	0.1865	C	-4.1114	1.0436	-0.3585	H	1.6514	2.7905	0.7632
C	-1.7251	-2.4434	0.0178	C	-3.5498	2.2683	-0.2164	H	-5.1875	0.9307	-0.5329
C	-3.1220	-2.5494	-0.1553	C	-2.1392	2.4130	0.0157	H	-4.1600	3.1775	-0.2682
C	-3.8967	-1.4243	-0.3043	H	4.9776	2.3256	-0.8905				
C	0.9417	0.2082	0.0735	H	6.2849	0.2774	-0.3777				

Table 3.267: Table of thermodynamic data as a function of temperature for Dibenzo[*a,ghi*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-46.009	415.372	415.372	∞
100	96.512	331.766	732.489	-40.072	439.342	479.149	-250.277
200	200.663	428.902	556.218	-25.463	426.617	524.040	-136.862
250	260.473	480.063	535.838	-13.944	420.668	549.083	-114.722
298.15	318.542	530.920	530.920	0.000	415.372	574.310	-100.615
300	320.744	532.898	530.927	0.591	415.176	575.294	-100.166
350	378.628	586.732	535.046	18.090	410.286	602.378	-89.898
400	432.312	640.849	544.890	38.384	406.029	630.109	-82.282
450	480.963	694.627	558.545	61.237	402.327	658.346	-76.417
500	524.463	747.598	574.810	86.394	399.102	686.989	-71.768
600	597.398	849.930	612.210	142.632	393.809	745.089	-64.864
700	655.003	946.516	653.140	205.363	389.876	803.971	-59.992
800	701.102	1037.099	695.536	273.250	387.146	863.317	-56.368
900	738.572	1121.914	738.251	345.297	385.465	922.935	-53.565
1000	769.445	1201.379	780.633	420.746	384.688	982.703	-51.330
1100	795.163	1275.957	822.308	499.014	384.639	1042.522	-49.504
1200	816.778	1346.098	863.064	579.642	385.195	1102.300	-47.981
1300	835.081	1412.218	902.788	662.259	386.191	1162.023	-46.690
1400	850.683	1474.690	941.428	746.568	387.512	1221.661	-45.580
1500	864.062	1533.849	978.968	832.322	389.086	1281.197	-44.614
1600	875.599	1589.992	1015.417	919.319	390.796	1340.614	-43.766
1700	885.599	1643.382	1050.799	1007.391	392.578	1399.899	-43.013
1800	894.311	1694.254	1085.145	1096.396	394.363	1459.139	-42.342
1900	901.937	1742.815	1118.491	1186.217	396.126	1518.231	-41.738
2000	908.642	1789.253	1150.876	1276.753	397.818	1577.256	-41.193
2100	914.562	1833.732	1182.342	1367.919	399.368	1636.187	-40.697
2200	919.811	1876.401	1212.927	1459.643	400.777	1695.049	-40.245
2300	924.484	1917.393	1242.670	1551.862	402.041	1753.850	-39.830
2400	928.658	1956.829	1271.611	1644.523	403.095	1812.554	-39.448
2500	932.401	1994.815	1299.784	1737.579	403.951	1871.325	-39.098
2600	935.767	2031.452	1327.224	1830.991	404.577	1929.956	-38.772
2700	938.805	2066.826	1353.966	1924.722	404.976	1988.637	-38.472
2800	941.555	2101.018	1380.039	2018.742	405.125	2047.327	-38.193
2900	944.051	2134.103	1405.474	2113.025	404.998	2105.966	-37.932
3000	946.323	2166.147	1430.298	2207.545	404.635	2164.640	-37.689
3100	948.397	2197.211	1454.539	2302.283	403.965	2223.256	-37.461
3200	950.293	2227.352	1478.221	2397.219	403.027	2281.969	-37.249
3300	952.033	2256.621	1501.367	2492.336	401.804	2340.753	-37.050
3400	953.631	2285.066	1524.001	2587.620	400.270	2399.495	-36.863
3500	955.104	2312.731	1546.143	2683.058	398.431	2458.270	-36.687
3600	956.463	2339.656	1567.812	2778.637	396.307	2517.186	-36.523
3700	957.719	2365.880	1589.029	2874.347	393.869	2576.179	-36.368
3800	958.883	2391.436	1609.810	2970.178	391.093	2635.187	-36.222
3900	959.964	2416.358	1630.173	3066.121	388.017	2694.222	-36.084
4000	960.968	2440.675	1650.132	3162.168	384.626	2753.472	-35.956
4100	961.904	2464.415	1669.705	3258.313	380.888	2812.741	-35.834
4200	962.776	2487.605	1688.903	3354.547	376.827	2872.097	-35.719
4300	963.591	2510.269	1707.742	3450.866	372.432	2931.468	-35.610
4400	964.354	2532.431	1726.234	3547.264	367.711	2991.031	-35.507
4500	965.068	2554.111	1744.392	3643.735	362.677	3050.758	-35.412
4600	965.737	2575.329	1762.226	3740.276	357.282	3110.611	-35.321
4700	966.367	2596.105	1779.748	3836.881	351.539	3170.476	-35.235
4800	966.958	2616.457	1796.968	3933.548	345.493	3230.567	-35.155
4900	967.515	2636.401	1813.896	4030.272	339.073	3290.658	-35.078
5000	968.040	2655.952	1830.542	4127.050	332.368	3351.061	-35.008

3.268. Naphtho[1,2,3,4-*ghi*]perylene



Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 190-84-1
Point Group: C_{2v}

Length: 13.76 Å
Width: 11.65 Å
Breadth: 3.894 Å
L/B Ratio: 1.182

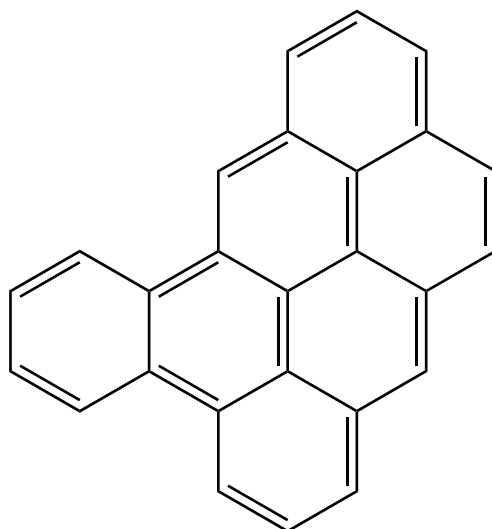
Cartesian coordinates:

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C	3.5679	-2.8405	0.0000	C	-2.5577	0.6961	0.0000	H	-0.1036	4.6291	0.0000
C	3.5727	-1.4379	0.0000	C	-3.7957	1.3791	0.0000	H	-2.2515	3.3762	0.0000
C	2.3863	-0.7228	0.0000	C	-4.9837	0.6880	0.0000	H	-2.2318	-3.3893	0.0000
C	-0.1131	3.5332	0.0000	C	-4.9796	-0.7171	0.0000	H	-0.0766	-4.6297	0.0000
C	-1.2866	2.8463	0.0000	C	-3.7876	-1.4013	0.0000	H	-3.7879	2.4798	0.0000
C	-0.1029	0.7185	0.0000	C	1.1353	2.8391	0.0000	H	-5.9373	1.2258	0.0000
C	-1.3080	1.4182	0.0000	C	1.1406	1.4298	0.0000	H	-5.9300	-1.2605	0.0000
C	1.1519	-2.8324	0.0000	C	2.3821	0.7367	0.0000	H	-3.7733	-2.5019	0.0000
C	1.1490	-1.4231	0.0000	C	3.5642	1.4587	0.0000	H	4.5230	0.9174	0.0000
C	-0.0987	-0.7191	0.0000	C	3.5512	2.8613	0.0000	H	4.5016	3.4053	0.0000
C	-1.2997	-1.4258	0.0000	C	2.3584	3.5458	0.0000	H	2.3429	4.6415	0.0000
C	-1.2700	-2.8537	0.0000	H	2.3701	-4.6277	0.0000				
C	-0.0924	-3.5338	0.0000	H	4.5215	-3.3789	0.0000				

Table 3.268: Table of thermodynamic data as a function of temperature for Naphtho[1,2,3,4-*ghi*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-46.336	391.987	391.987	∞
100	98.615	331.430	733.266	-40.184	415.846	455.687	-238.021
200	201.105	429.532	556.757	-25.445	403.250	500.547	-130.727
250	260.240	480.715	536.400	-13.921	397.306	525.558	-109.807
298.15	317.874	531.491	531.491	0.000	391.987	550.755	-96.488
300	320.063	533.464	531.497	0.590	391.790	551.738	-96.064
350	377.688	587.172	535.607	18.048	386.859	578.797	-86.379
400	431.242	641.153	545.427	38.290	382.551	606.510	-79.200
450	479.846	694.803	559.049	61.089	378.794	634.734	-73.677
500	523.346	747.655	575.276	86.190	375.513	663.371	-69.300
600	596.342	849.789	612.590	142.319	370.112	721.476	-62.809
700	654.030	946.218	653.435	204.948	366.077	780.380	-58.231
800	700.208	1036.676	695.748	272.743	363.254	839.763	-54.830
900	737.749	1121.390	738.386	344.703	361.486	899.428	-52.200
1000	768.687	1200.771	780.698	420.073	360.630	959.253	-50.105
1100	794.463	1275.280	822.309	498.269	360.509	1019.136	-48.394
1200	816.133	1345.363	863.006	578.829	360.997	1078.985	-46.966
1300	834.487	1411.434	902.676	661.385	361.932	1138.784	-45.756
1400	850.135	1473.863	941.266	745.636	363.196	1198.502	-44.716
1500	863.556	1532.986	978.761	831.338	364.717	1258.123	-43.811
1600	875.131	1589.097	1015.168	918.286	366.378	1317.628	-43.015
1700	885.167	1642.460	1050.511	1006.313	368.115	1377.004	-42.309
1800	893.911	1693.308	1084.821	1095.276	369.859	1436.338	-41.681
1900	901.565	1741.848	1118.133	1185.059	371.583	1495.525	-41.114
2000	908.297	1788.268	1150.488	1275.559	373.239	1554.648	-40.602
2100	914.241	1832.730	1181.925	1366.692	374.756	1613.678	-40.137
2200	919.513	1875.385	1212.483	1458.385	376.134	1672.640	-39.713
2300	924.205	1916.364	1242.201	1550.575	377.369	1731.544	-39.324
2400	928.398	1955.788	1271.118	1643.209	378.396	1790.351	-38.965
2500	932.157	1993.765	1299.269	1736.240	379.227	1849.227	-38.637
2600	935.539	2030.392	1326.689	1829.628	379.829	1907.964	-38.331
2700	938.591	2065.758	1353.411	1923.337	380.206	1966.751	-38.048
2800	941.353	2099.943	1379.466	2017.336	380.335	2025.548	-37.786
2900	943.861	2133.021	1404.883	2111.599	380.187	2084.295	-37.541
3000	946.144	2165.058	1429.691	2206.101	379.806	2143.077	-37.314
3100	948.227	2196.116	1453.916	2300.821	379.119	2201.803	-37.099
3200	950.133	2226.252	1477.583	2395.741	378.164	2260.625	-36.900
3300	951.881	2255.516	1500.715	2490.843	376.926	2319.520	-36.714
3400	953.488	2283.957	1523.336	2586.112	375.377	2378.372	-36.538
3500	954.967	2311.618	1545.465	2681.536	373.524	2437.258	-36.373
3600	956.333	2338.539	1567.122	2777.102	371.387	2496.286	-36.219
3700	957.596	2364.759	1588.327	2872.799	368.936	2555.391	-36.075
3800	958.766	2390.312	1609.097	2968.618	366.148	2614.511	-35.938
3900	959.852	2415.231	1629.449	3064.549	363.061	2673.658	-35.809
4000	960.861	2439.545	1649.399	3160.586	359.659	2733.022	-35.689
4100	961.801	2463.283	1668.961	3256.719	355.910	2792.403	-35.575
4200	962.678	2486.471	1688.151	3352.944	351.839	2851.873	-35.467
4300	963.498	2509.133	1706.981	3449.253	347.434	2911.357	-35.365
4400	964.264	2531.292	1725.465	3545.641	342.704	2971.034	-35.270
4500	964.982	2552.970	1743.614	3642.104	337.661	3030.875	-35.181
4600	965.655	2574.187	1761.440	3738.636	332.258	3090.842	-35.097
4700	966.287	2594.961	1778.954	3835.234	326.507	3150.821	-35.017
4800	966.882	2615.311	1796.167	3931.892	320.453	3211.027	-34.942
4900	967.442	2635.253	1813.088	4028.609	314.025	3271.233	-34.871
5000	967.970	2654.804	1829.728	4125.380	307.313	3331.750	-34.806

3.269. Benzo[qr]naphtho[3,2,1,8-defg]chrysene



Other names: Benzo[*e*]anthanthrene

Formula: C₂₆H₁₄

Mass: 326.389 g/mol

CAS Number: 75459-05-1

Point Group: C_s

Length: 13.81 Å

Width: 11.13 Å

Breadth: 3.886 Å

L/B Ratio: 1.241

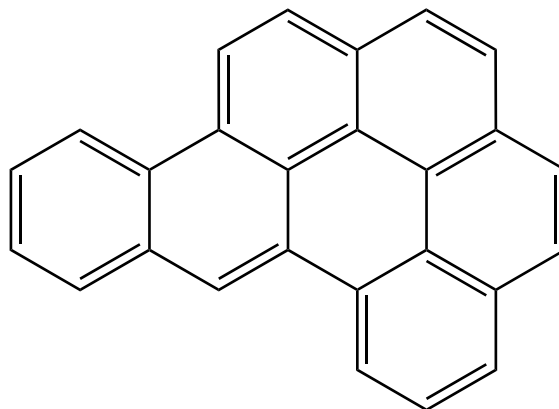
Cartesian coordinates:

C	4.7156	0.8964	0.0000	C	2.3552	0.3368	0.0000	H	2.8140	3.7301	0.0000
C	4.3846	2.2575	0.0000	C	1.3124	-0.6379	0.0000	H	0.4094	3.1716	0.0000
C	3.0666	2.6639	0.0000	C	1.6462	-2.0315	0.0000	H	-4.4689	-1.5148	0.0000
C	2.0287	1.7091	0.0000	C	3.0448	-2.4080	0.0000	H	-3.8627	-3.9239	0.0000
C	0.6574	2.0978	0.0000	C	4.0232	-1.4807	0.0000	H	-1.4767	-4.6217	0.0000
C	-0.3499	1.1667	0.0000	C	3.7167	-0.0666	0.0000	H	0.8936	-4.0450	0.0000
C	-2.4312	-0.8320	0.0000	C	-2.7705	0.5880	0.0000	H	3.2819	-3.4784	0.0000
C	-3.4086	-1.8110	0.0000	C	-1.7564	1.5619	0.0000	H	5.0797	-1.7726	0.0000
C	-3.0654	-3.1732	0.0000	C	-2.1120	2.9188	0.0000	H	-1.3123	3.6755	0.0000
C	-1.7477	-3.5598	0.0000	C	-3.4410	3.3061	0.0000	H	-3.7028	4.3691	0.0000
C	-0.0278	-0.2333	0.0000	C	-4.4465	2.3400	0.0000	H	-5.4983	2.6439	0.0000
C	-1.0606	-1.2160	0.0000	C	-4.1123	0.9967	0.0000	H	-4.8996	0.2270	0.0000
C	-0.7194	-2.5865	0.0000	H	5.7688	0.5937	0.0000				
C	0.6480	-2.9758	0.0000	H	5.1869	3.0030	0.0000				

Table 3.269: Table of thermodynamic data as a function of temperature for Benzo[*qr*]naphtho[3,2,1,8-*defg*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.132	398.896	398.896	∞
100	97.579	335.675	736.353	-40.068	422.871	462.287	-241.469
200	200.550	433.202	560.249	-25.409	410.195	506.758	-132.349
250	259.892	484.285	539.917	-13.908	404.229	531.588	-111.067
298.15	317.648	535.012	535.012	0.000	398.896	556.614	-97.514
300	319.840	536.983	535.018	0.590	398.699	557.591	-97.083
350	377.523	590.662	539.125	18.038	393.758	584.475	-87.226
400	431.097	644.623	548.941	38.273	389.442	612.013	-79.919
450	479.705	698.255	562.557	61.064	385.679	640.065	-74.295
500	523.208	751.093	578.777	86.158	382.390	668.529	-69.839
600	596.221	853.203	616.079	142.274	376.976	726.292	-63.228
700	653.942	949.615	656.911	204.893	372.930	784.855	-58.565
800	700.160	1040.065	699.214	272.680	370.101	843.899	-55.100
900	737.739	1124.775	741.844	344.638	368.330	903.226	-52.421
1000	768.708	1204.157	784.148	420.009	367.475	962.712	-50.286
1100	794.509	1278.669	825.753	498.208	367.357	1022.256	-48.542
1200	816.196	1348.757	866.446	578.774	367.851	1081.766	-47.087
1300	834.561	1414.833	906.112	661.336	368.793	1141.226	-45.854
1400	850.216	1477.268	944.700	745.596	370.064	1200.604	-44.794
1500	863.641	1536.397	982.193	831.305	371.594	1259.884	-43.872
1600	875.218	1592.513	1018.599	918.262	373.264	1319.047	-43.062
1700	885.254	1645.881	1053.942	1006.298	375.009	1378.081	-42.342
1800	893.996	1696.734	1088.251	1095.270	376.761	1437.073	-41.702
1900	901.649	1745.280	1121.564	1185.061	378.494	1495.917	-41.125
2000	908.377	1791.703	1153.918	1275.569	380.158	1554.697	-40.604
2100	914.319	1836.170	1185.355	1366.710	381.683	1613.383	-40.130
2200	919.587	1878.828	1215.914	1458.410	383.069	1672.001	-39.698
2300	924.276	1919.810	1245.633	1550.608	384.311	1730.560	-39.301
2400	928.466	1959.237	1274.550	1643.249	385.345	1789.023	-38.936
2500	932.222	1997.217	1302.702	1736.287	386.183	1847.554	-38.602
2600	935.601	2033.846	1330.123	1829.681	386.791	1905.945	-38.290
2700	938.650	2069.214	1356.845	1923.396	387.174	1964.387	-38.003
2800	941.409	2103.401	1382.901	2017.401	387.308	2022.838	-37.736
2900	943.915	2136.481	1408.319	2111.669	387.167	2081.239	-37.486
3000	946.195	2168.520	1433.128	2206.177	386.791	2139.675	-37.254
3100	948.276	2199.580	1457.354	2300.902	386.108	2198.054	-37.036
3200	950.180	2229.717	1481.022	2395.826	385.158	2256.530	-36.833
3300	951.925	2258.983	1504.155	2490.932	383.925	2315.078	-36.644
3400	953.530	2287.425	1526.776	2586.206	382.381	2373.584	-36.465
3500	955.007	2315.087	1548.906	2681.634	380.531	2432.123	-36.297
3600	956.371	2342.010	1570.564	2777.204	378.398	2490.803	-36.140
3700	957.632	2368.231	1591.770	2872.905	375.951	2549.561	-35.993
3800	958.801	2393.785	1612.541	2968.727	373.167	2608.335	-35.853
3900	959.885	2418.704	1632.894	3064.662	370.083	2667.134	-35.722
4000	960.894	2443.019	1652.844	3160.702	366.684	2726.150	-35.599
4100	961.832	2466.758	1672.407	3256.839	362.938	2785.185	-35.483
4200	962.708	2489.947	1691.597	3353.066	358.871	2844.307	-35.373
4300	963.526	2512.609	1710.428	3449.378	354.469	2903.443	-35.269
4400	964.291	2534.769	1728.912	3545.770	349.741	2962.773	-35.172
4500	965.008	2556.448	1747.062	3642.235	344.701	3022.266	-35.081
4600	965.680	2577.665	1764.889	3738.770	339.300	3081.885	-34.995
4700	966.312	2598.440	1782.404	3835.370	333.552	3141.516	-34.913
4800	966.906	2618.790	1799.617	3932.031	327.500	3201.374	-34.837
4900	967.465	2638.733	1816.539	4028.750	321.075	3261.232	-34.764
5000	967.992	2658.284	1833.179	4125.523	314.365	3321.402	-34.698

3.270. Dibenzo[*b,ghi*]perylene



Other names: 1.12,4.5-Dibenzoperylene

Formula: C₂₆H₁₄

Mass: 326.389 g/mol

CAS Number: 5869-30-7

Point Group: C_s

Length: 14.27 Å

Width: 11.12 Å

Breadth: 3.886 Å

L/B Ratio: 1.284

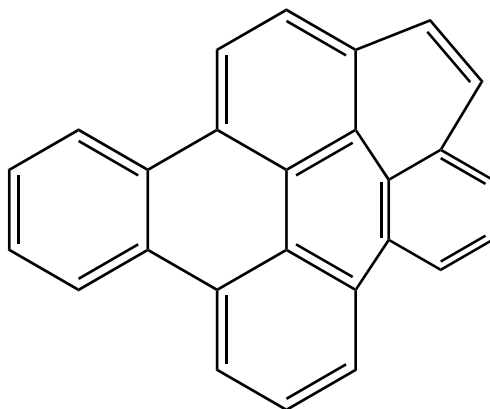
Cartesian coordinates:

C	5.4241	-0.1406	0.0000	C	1.7987	-1.0822	0.0000	H	4.0249	2.9708	0.0000
C	5.3323	1.2659	0.0000	C	0.5561	-0.4382	0.0000	H	4.3430	-2.0074	0.0000
C	4.1043	1.8778	0.0000	C	-0.8257	1.6457	0.0000	H	1.5855	2.8335	0.0000
C	4.2869	-0.9081	0.0000	C	-0.9458	3.0275	0.0000	H	-3.9128	-3.3602	0.0000
C	3.0068	-0.3023	0.0000	C	-2.2063	3.6390	0.0000	H	-1.6953	-4.4789	0.0000
C	2.9178	1.1025	0.0000	C	-3.3534	2.8764	0.0000	H	0.7517	-4.3483	0.0000
C	1.6405	1.7326	0.0000	C	-2.0013	0.8506	0.0000	H	2.8381	-2.9870	0.0000
C	0.4840	0.9968	0.0000	C	-3.2668	1.4687	0.0000	H	-0.0338	3.6443	0.0000
C	-2.9891	-2.7703	0.0000	C	-4.4470	0.6554	0.0000	H	-2.2708	4.7321	0.0000
C	-1.7698	-3.3854	0.0000	C	-4.3598	-0.6998	0.0000	H	-4.3400	3.3533	0.0000
C	-0.6415	-1.2192	0.0000	C	-3.0847	-1.3512	0.0000	H	-5.4220	1.1561	0.0000
C	-0.5704	-2.6200	0.0000	C	-1.9178	-0.5804	0.0000	H	-5.2621	-1.3219	0.0000
C	0.7066	-3.2533	0.0000	H	6.4115	-0.6137	0.0000				
C	1.8466	-2.5082	0.0000	H	6.2500	1.8629	0.0000				

Table 3.270: Table of thermodynamic data as a function of temperature for Dibenzo[*b,ghi*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-46.285	383.088	383.088	∞
100	98.209	337.625	739.078	-40.145	406.984	446.206	-233.069
200	200.895	435.452	562.678	-25.445	394.351	490.463	-128.093
250	260.258	486.614	542.318	-13.926	388.402	515.179	-107.639
298.15	318.041	537.407	537.407	0.000	383.088	540.092	-94.620
300	320.234	539.381	537.413	0.590	382.891	541.064	-94.206
350	377.937	593.122	541.525	18.059	377.971	567.826	-84.742
400	431.520	647.139	551.352	38.315	373.676	595.240	-77.729
450	480.127	700.821	564.982	61.127	369.933	623.165	-72.334
500	523.621	753.703	581.219	86.242	366.666	651.500	-68.060
600	596.602	855.885	618.555	142.398	361.291	708.998	-61.722
700	654.287	952.354	659.421	205.053	357.282	767.290	-57.255
800	700.469	1042.847	701.755	272.873	354.485	826.057	-53.935
900	738.016	1127.592	744.414	344.860	352.744	885.104	-51.369
1000	768.956	1207.002	786.745	420.257	351.915	944.307	-49.325
1100	794.732	1281.536	828.373	498.480	351.820	1003.566	-47.654
1200	816.397	1351.642	869.087	579.067	352.336	1062.788	-46.261
1300	834.743	1417.733	908.773	661.649	353.296	1121.959	-45.080
1400	850.382	1480.182	947.378	745.925	354.585	1181.046	-44.064
1500	863.792	1539.321	984.887	831.651	356.131	1240.034	-43.181
1600	875.355	1595.447	1021.308	918.622	357.815	1298.904	-42.404
1700	885.379	1648.823	1056.664	1006.671	359.573	1357.645	-41.714
1800	894.111	1699.683	1090.986	1095.655	361.338	1416.342	-41.100
1900	901.754	1748.234	1124.310	1185.457	363.081	1474.891	-40.547
2000	908.475	1794.663	1156.675	1275.975	364.756	1533.375	-40.047
2100	914.409	1839.134	1188.122	1367.125	366.290	1591.764	-39.592
2200	919.671	1881.796	1218.689	1458.834	367.684	1650.086	-39.177
2300	924.354	1922.782	1248.417	1551.040	368.935	1708.349	-38.797
2400	928.538	1962.212	1277.342	1643.689	369.976	1766.514	-38.446
2500	932.289	2000.195	1305.501	1736.733	370.821	1824.747	-38.125
2600	935.663	2036.827	1332.929	1830.134	371.436	1882.840	-37.826
2700	938.708	2072.197	1359.658	1923.855	371.825	1940.984	-37.550
2800	941.465	2106.386	1385.720	2017.866	371.965	1999.137	-37.294
2900	943.966	2139.468	1411.144	2112.139	371.828	2057.240	-37.054
3000	946.244	2171.509	1435.958	2206.652	371.458	2115.377	-36.831
3100	948.322	2202.570	1460.189	2301.382	370.779	2173.457	-36.622
3200	950.223	2232.709	1483.862	2396.310	369.834	2231.634	-36.427
3300	951.966	2261.976	1507.000	2491.421	368.605	2289.882	-36.245
3400	953.568	2290.419	1529.625	2586.699	367.065	2348.089	-36.073
3500	955.044	2318.082	1551.759	2682.130	365.219	2406.328	-35.912
3600	956.406	2345.006	1573.421	2777.704	363.090	2464.709	-35.761
3700	957.666	2371.228	1594.631	2873.408	360.646	2523.168	-35.620
3800	958.832	2396.783	1615.405	2969.234	357.865	2581.641	-35.486
3900	959.915	2421.703	1635.761	3065.172	354.784	2640.141	-35.360
4000	960.922	2446.019	1655.715	3161.214	351.388	2698.857	-35.243
4100	961.860	2469.758	1675.281	3257.354	347.645	2757.592	-35.131
4200	962.734	2492.947	1694.475	3353.584	343.580	2816.413	-35.027
4300	963.551	2515.610	1713.308	3449.899	339.181	2875.250	-34.927
4400	964.315	2537.771	1731.795	3546.293	334.456	2934.280	-34.834
4500	965.031	2559.450	1749.948	3642.760	329.418	2993.473	-34.747
4600	965.702	2580.668	1767.777	3739.297	324.019	3052.792	-34.665
4700	966.333	2601.443	1785.294	3835.900	318.273	3112.122	-34.587
4800	966.926	2621.794	1802.510	3932.563	312.224	3171.680	-34.514
4900	967.484	2641.737	1819.434	4029.284	305.800	3231.237	-34.445
5000	968.010	2661.288	1836.077	4126.059	299.092	3291.106	-34.381

3.271. Dibenzo[*b,pqr*]perylene



Other names: 1.12,2.3-Dibenzoperylene
Dibenzo[*e,ghi*]perylene

Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 190-95-4
Point Group: C_s

Length: 13.80 Å
Width: 10.41 Å
Breadth: 3.891 Å
L/B Ratio: 1.325

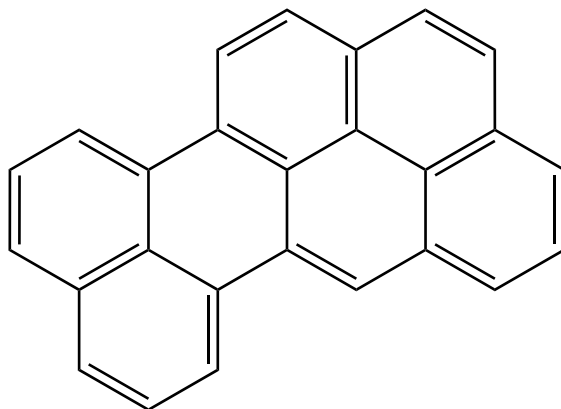
Cartesian coordinates:

C	4.9935	-1.2627	0.0000	C	0.3828	0.9236	0.0000	H	4.3136	2.0778	0.0000
C	5.2169	0.1186	0.0000	C	-0.7125	1.8176	0.0000	H	3.5180	-2.8367	0.0000
C	4.1468	0.9896	0.0000	C	-2.0747	1.2975	0.0000	H	2.9305	3.2049	0.0000
C	3.7034	-1.7517	0.0000	C	-3.1772	2.1456	0.0000	H	0.9941	4.7695	0.0000
C	2.5995	-0.8781	0.0000	C	-4.4754	1.6307	0.0000	H	-1.3342	3.8817	0.0000
C	2.8237	0.5094	0.0000	C	-4.6878	0.2658	0.0000	H	-0.4711	-4.3556	0.0000
C	1.6982	1.4300	0.0000	C	-2.2820	-0.1032	0.0000	H	1.8518	-3.4698	0.0000
C	1.9004	2.8169	0.0000	C	-3.5945	-0.6179	0.0000	H	-3.0143	3.2344	0.0000
C	0.8239	3.6878	0.0000	C	-3.7939	-2.0408	0.0000	H	-5.3271	2.3190	0.0000
C	-0.4756	3.1925	0.0000	C	-2.7388	-2.8908	0.0000	H	-5.7068	-0.1374	0.0000
C	1.2414	-1.3929	0.0000	C	-1.3924	-2.3924	0.0000	H	-4.8228	-2.4187	0.0000
C	-0.2912	-3.2745	0.0000	C	-1.1661	-1.0063	0.0000	H	-2.8888	-3.9765	0.0000
C	0.9912	-2.7831	0.0000	H	5.8441	-1.9519	0.0000				
C	0.1617	-0.5022	0.0000	H	6.2415	0.5044	0.0000				

Table 3.271: Table of thermodynamic data as a function of temperature for Dibenzo[*b,pqr*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-46.642	383.679	383.679	∞
100	99.745	342.738	745.932	-40.319	407.402	446.112	-233.020
200	201.752	441.440	568.924	-25.497	394.890	489.806	-127.921
250	260.758	492.753	548.530	-13.944	388.975	514.218	-107.438
298.15	318.315	543.613	543.613	0.000	383.679	538.833	-94.399
300	320.503	545.589	543.619	0.591	383.483	539.794	-93.985
350	378.086	599.361	547.734	18.069	378.573	566.245	-84.506
400	431.618	653.394	557.565	38.331	374.284	593.346	-77.481
450	480.207	707.087	571.201	61.148	370.546	620.958	-72.077
500	523.693	759.976	587.443	86.267	367.282	648.979	-67.797
600	596.659	862.171	624.788	142.429	361.914	705.850	-61.448
700	654.314	958.646	665.662	205.089	357.909	763.513	-56.973
800	700.460	1049.140	708.003	272.910	355.113	821.651	-53.647
900	737.971	1133.882	750.666	344.894	353.369	880.068	-51.077
1000	768.883	1213.285	793.001	420.285	352.534	938.643	-49.029
1100	794.637	1287.812	834.631	498.499	352.431	997.273	-47.356
1200	816.287	1357.909	875.346	579.076	352.936	1055.868	-45.960
1300	834.623	1423.991	915.032	661.646	353.885	1114.413	-44.777
1400	850.257	1486.430	953.637	745.910	355.161	1172.874	-43.760
1500	863.666	1545.561	991.145	831.623	356.694	1231.238	-42.875
1600	875.230	1601.679	1027.565	918.582	358.366	1289.485	-42.097
1700	885.256	1655.047	1062.919	1006.618	360.112	1347.603	-41.406
1800	893.992	1705.900	1097.239	1095.590	361.864	1405.678	-40.791
1900	901.640	1754.445	1130.561	1185.380	363.596	1463.605	-40.236
2000	908.365	1800.868	1162.924	1275.888	365.260	1521.468	-39.736
2100	914.304	1845.334	1194.368	1367.027	366.783	1579.238	-39.281
2200	919.570	1887.991	1224.934	1458.726	368.167	1636.940	-38.865
2300	924.258	1928.973	1254.659	1550.922	369.408	1694.583	-38.484
2400	928.447	1968.399	1283.582	1643.561	370.440	1752.129	-38.133
2500	932.203	2006.378	1311.739	1736.597	371.276	1809.744	-37.812
2600	935.581	2043.006	1339.164	1829.989	371.882	1867.219	-37.512
2700	938.631	2078.374	1365.891	1923.702	372.263	1924.745	-37.236
2800	941.391	2112.560	1391.951	2017.705	372.396	1982.281	-36.979
2900	943.896	2145.639	1417.373	2111.972	372.252	2039.766	-36.739
3000	946.177	2177.678	1442.185	2206.477	371.874	2097.286	-36.516
3100	948.258	2208.737	1466.414	2301.200	371.190	2154.749	-36.307
3200	950.162	2238.874	1490.085	2396.123	370.238	2212.310	-36.112
3300	951.908	2268.139	1513.221	2491.228	369.003	2269.942	-35.929
3400	953.513	2296.580	1535.845	2586.500	367.457	2327.532	-35.757
3500	954.992	2324.242	1557.977	2681.926	365.606	2385.156	-35.596
3600	956.356	2351.164	1579.638	2777.494	363.472	2442.921	-35.445
3700	957.618	2377.385	1600.846	2873.194	361.023	2500.763	-35.304
3800	958.787	2402.938	1621.619	2969.015	358.237	2558.621	-35.170
3900	959.871	2427.858	1641.973	3064.948	355.152	2616.506	-35.043
4000	960.880	2452.172	1661.926	3160.986	351.752	2674.606	-34.926
4100	961.819	2475.911	1681.491	3257.122	348.004	2732.726	-34.815
4200	962.696	2499.099	1700.683	3353.348	343.936	2790.932	-34.710
4300	963.514	2521.761	1719.515	3449.659	339.532	2849.154	-34.610
4400	964.280	2543.921	1738.000	3546.049	334.804	2907.568	-34.517
4500	964.997	2565.599	1756.152	3642.514	329.763	2966.146	-34.429
4600	965.669	2586.816	1773.980	3739.047	324.360	3024.850	-34.348
4700	966.301	2607.591	1791.496	3835.646	318.611	3083.566	-34.269
4800	966.895	2627.941	1808.711	3932.306	312.558	3142.509	-34.197
4900	967.455	2647.883	1825.634	4029.024	306.132	3201.452	-34.127
5000	967.982	2667.434	1842.275	4125.796	299.421	3260.706	-34.064

3.272. Naphtho[8,1,2-*bcd*]perylene



Formula: C₂₆H₁₄
Mass: 326.389 g/mol
CAS Number: 188-89-6
Point Group: C_s

Length: 14.28 Å
Width: 10.32 Å
Breadth: 3.889 Å
L/B Ratio: 1.384

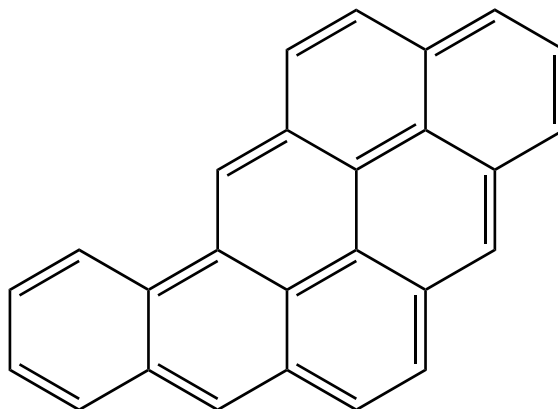
Cartesian coordinates:

C	4.5266	-1.8066	0.0000	C	0.2040	0.9547	0.0000	H	2.8476	-3.1879	0.0000
C	4.9287	-0.4972	0.0000	C	-0.7457	1.9339	0.0000	H	5.4421	2.1410	0.0000
C	3.1562	-2.1311	0.0000	C	-2.1474	1.6255	0.0000	H	3.7404	3.9564	0.0000
C	3.9656	0.5456	0.0000	C	-3.1198	2.6314	0.0000	H	1.3177	3.4051	0.0000
C	4.3716	1.9070	0.0000	C	-4.4689	2.2992	0.0000	H	-1.3169	-4.1786	0.0000
C	3.4347	2.9050	0.0000	C	-4.8742	0.9696	0.0000	H	1.1010	-3.6009	0.0000
C	2.0604	2.5923	0.0000	C	-1.5621	-0.7662	0.0000	H	-0.4405	2.9930	0.0000
C	2.1922	-1.1435	0.0000	C	-2.5496	0.2712	0.0000	H	-2.8124	3.6831	0.0000
C	2.5906	0.2267	0.0000	C	-3.9244	-0.0564	0.0000	H	-5.2220	3.0943	0.0000
C	1.6294	1.2816	0.0000	C	-4.3107	-1.4440	0.0000	H	-5.9414	0.7205	0.0000
C	0.7683	-1.4698	0.0000	C	-3.3798	-2.4256	0.0000	H	-5.3810	-1.6800	0.0000
C	-1.0048	-3.1281	0.0000	C	-1.9731	-2.1175	0.0000	H	-3.6737	-3.4816	0.0000
C	0.3408	-2.8041	0.0000	H	5.2647	-2.6154	0.0000				
C	-0.1855	-0.4385	0.0000	H	5.9931	-0.2367	0.0000				

Table 3.272: Table of thermodynamic data as a function of temperature for Naphtho[8,1,2-*bcd*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.293	406.261	406.261	∞
100	97.949	341.038	742.442	-40.140	430.163	469.043	-244.998
200	200.876	438.752	566.028	-25.455	417.514	512.967	-133.970
250	260.368	489.925	545.659	-13.934	411.568	537.518	-112.306
298.15	318.235	540.745	540.745	0.000	406.261	562.270	-98.505
300	320.431	542.720	540.751	0.591	406.065	563.236	-98.066
350	378.184	596.496	544.866	18.070	401.156	589.831	-88.026
400	431.792	650.548	554.699	38.340	396.874	617.075	-80.580
450	480.408	704.263	568.338	61.166	393.145	644.828	-74.848
500	523.900	757.174	584.585	86.295	389.892	672.991	-70.305
600	596.862	859.406	621.943	142.478	384.544	730.139	-63.563
700	654.518	955.913	662.831	205.157	380.560	788.077	-58.806
800	700.672	1046.434	705.185	272.999	377.785	846.487	-55.269
900	738.193	1131.201	747.863	345.005	376.062	905.174	-52.534
1000	769.111	1210.629	790.210	420.418	375.250	964.015	-50.354
1100	794.868	1285.177	831.854	498.655	375.170	1022.910	-48.573
1200	816.516	1355.295	872.582	579.255	375.698	1081.767	-47.087
1300	834.849	1421.395	912.280	661.848	376.670	1140.573	-45.828
1400	850.475	1483.850	950.897	746.135	377.968	1199.293	-44.745
1500	863.875	1542.996	988.416	831.869	379.523	1257.914	-43.804
1600	875.430	1599.127	1024.847	918.849	381.215	1316.417	-42.976
1700	885.447	1652.507	1060.211	1006.904	382.981	1374.789	-42.241
1800	894.172	1703.371	1094.540	1095.895	384.751	1433.117	-41.587
1900	901.810	1751.925	1127.871	1185.702	386.501	1491.298	-40.998
2000	908.526	1798.356	1160.243	1276.226	388.181	1549.412	-40.466
2100	914.456	1842.830	1191.696	1367.381	389.720	1607.433	-39.982
2200	919.713	1885.494	1222.269	1459.095	391.118	1665.385	-39.540
2300	924.393	1926.482	1252.002	1551.305	392.373	1723.277	-39.136
2400	928.574	1965.914	1280.932	1643.957	393.418	1781.072	-38.763
2500	932.323	2003.898	1309.095	1737.005	394.267	1838.935	-38.422
2600	935.695	2040.531	1336.527	1830.409	394.884	1896.658	-38.104
2700	938.738	2075.902	1363.260	1924.133	395.277	1954.432	-37.810
2800	941.492	2110.093	1389.326	2018.147	395.419	2012.214	-37.538
2900	943.992	2143.175	1414.753	2112.423	395.286	2069.946	-37.283
3000	946.268	2175.217	1439.571	2206.938	394.917	2127.712	-37.046
3100	948.344	2206.279	1463.805	2301.670	394.242	2185.421	-36.823
3200	950.244	2236.418	1487.480	2396.601	393.298	2243.227	-36.616
3300	951.986	2265.686	1510.621	2491.714	392.071	2301.105	-36.423
3400	953.587	2294.130	1533.249	2586.993	390.533	2358.940	-36.240
3500	955.062	2321.793	1555.386	2682.427	388.689	2416.809	-36.068
3600	956.423	2348.718	1577.050	2778.002	386.561	2474.819	-35.908
3700	957.682	2374.940	1598.262	2873.708	384.120	2532.906	-35.757
3800	958.848	2400.495	1619.039	2969.535	381.340	2591.008	-35.615
3900	959.930	2425.416	1639.397	3065.475	378.260	2649.137	-35.480
4000	960.936	2449.732	1659.352	3161.519	374.866	2707.481	-35.355
4100	961.873	2473.472	1678.921	3257.660	371.124	2765.845	-35.237
4200	962.747	2496.661	1698.116	3353.891	367.061	2824.295	-35.125
4300	963.563	2519.325	1716.951	3450.207	362.663	2882.760	-35.018
4400	964.327	2541.486	1735.440	3546.602	357.939	2941.418	-34.918
4500	965.042	2563.165	1753.593	3643.071	352.902	3000.240	-34.825
4600	965.713	2584.383	1771.424	3739.609	347.504	3059.187	-34.737
4700	966.343	2605.158	1788.943	3836.212	341.760	3118.146	-34.654
4800	966.936	2625.510	1806.160	3932.876	335.711	3177.332	-34.576
4900	967.493	2645.453	1823.086	4029.598	329.289	3236.518	-34.501
5000	968.019	2665.004	1839.729	4126.374	322.581	3296.016	-34.433

3.273. Naphtho[7,8,1,2,3-*pqrst*]pentaphene



Other names: Benzo[*a*]anthanthrene

Formula: C₂₆H₁₄

Mass: 326.389 g/mol

CAS Number: 120835-55-4

Point Group: C_s

Length: 15.87 Å

Width: 10.44 Å

Breadth: 3.885 Å

L/B Ratio: 1.520

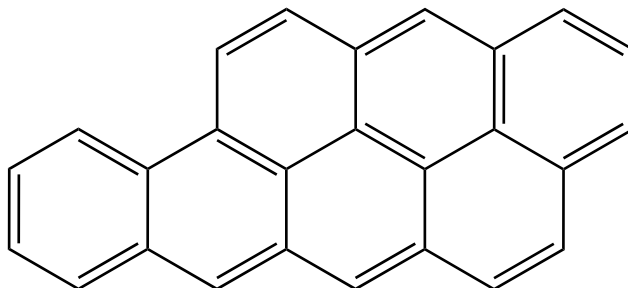
Cartesian coordinates:

C	5.0055	-1.9774	0.0000	C	1.5244	-0.5893	0.0000	H	5.7263	1.3558	0.0000
C	5.7656	-0.7928	0.0000	C	0.9108	0.6765	0.0000	H	3.0248	-2.8357	0.0000
C	5.1398	0.4300	0.0000	C	-3.3272	0.9788	0.0000	H	3.6955	2.6895	0.0000
C	3.6330	-1.9182	0.0000	C	-4.7322	1.0558	0.0000	H	1.6619	4.0557	0.0000
C	2.9646	-0.6722	0.0000	C	-5.4937	-0.0978	0.0000	H	-0.8071	4.2230	0.0000
C	3.7265	0.5116	0.0000	C	-4.8876	-1.3572	0.0000	H	-3.0084	3.1332	0.0000
C	3.0764	1.7838	0.0000	C	-2.7093	-0.2911	0.0000	H	1.2252	-2.7330	0.0000
C	1.7113	1.8716	0.0000	C	-3.5013	-1.4672	0.0000	H	-5.2167	2.0387	0.0000
C	1.0353	3.1561	0.0000	C	-2.8391	-2.7519	0.0000	H	-6.5868	-0.0290	0.0000
C	-0.3071	3.2474	0.0000	C	-1.4925	-2.8468	0.0000	H	-5.5078	-2.2605	0.0000
C	-1.1471	2.0642	0.0000	C	-0.6565	-1.6673	0.0000	H	-3.4685	-3.6493	0.0000
C	-2.5131	2.1544	0.0000	C	-1.2845	-0.3883	0.0000	H	-0.9954	-3.8237	0.0000
C	-0.5031	0.7767	0.0000	H	5.5175	-2.9451	0.0000				
C	0.7230	-1.7522	0.0000	H	6.8587	-0.8561	0.0000				

Table 3.273: Table of thermodynamic data as a function of temperature for Naphtho[7,8,1,2,3-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.108	398.899	398.899	∞
100	97.068	333.863	735.069	-40.121	422.821	462.418	-241.538
200	200.898	431.278	558.644	-25.473	410.134	507.082	-132.433
250	260.576	482.478	538.259	-13.945	404.194	532.005	-111.154
298.15	318.494	533.341	533.341	0.000	398.899	557.115	-97.602
300	320.690	535.318	533.347	0.591	398.703	558.095	-97.171
350	378.418	589.132	537.465	18.083	393.807	585.059	-87.313
400	431.970	643.211	547.304	38.363	389.535	612.670	-80.005
450	480.526	696.944	560.951	61.197	385.814	640.790	-74.379
500	523.969	749.865	577.205	86.330	382.565	669.318	-69.922
600	596.874	852.104	614.576	142.517	377.221	727.197	-63.307
700	654.518	948.611	655.473	205.197	373.237	785.865	-58.641
800	700.683	1039.133	697.835	273.039	370.462	845.005	-55.172
900	738.223	1123.903	740.517	345.047	368.742	904.422	-52.490
1000	769.160	1203.334	782.870	420.464	367.933	963.993	-50.353
1100	794.933	1277.888	824.518	498.707	367.859	1023.617	-48.607
1200	816.593	1348.012	865.250	579.314	368.394	1083.203	-47.150
1300	834.933	1414.118	904.953	661.915	369.374	1142.736	-45.915
1400	850.564	1476.581	943.573	746.210	370.682	1202.184	-44.853
1500	863.966	1535.732	981.096	831.954	372.245	1261.532	-43.930
1600	875.522	1591.869	1017.530	918.942	373.946	1320.761	-43.118
1700	885.537	1645.255	1052.898	1007.007	375.721	1379.859	-42.397
1800	894.260	1696.123	1087.231	1096.007	377.501	1438.912	-41.755
1900	901.895	1744.682	1120.565	1185.823	379.259	1497.816	-41.177
2000	908.607	1791.118	1152.941	1276.355	380.947	1556.655	-40.655
2100	914.534	1835.595	1184.396	1367.518	382.494	1615.399	-40.180
2200	919.788	1878.263	1214.973	1459.239	383.900	1674.074	-39.747
2300	924.465	1919.255	1244.708	1551.456	385.162	1732.690	-39.350
2400	928.643	1958.689	1273.641	1644.116	386.215	1791.207	-38.984
2500	932.388	1996.676	1301.808	1737.170	387.070	1849.793	-38.649
2600	935.757	2033.311	1329.242	1830.581	387.694	1908.238	-38.336
2700	938.796	2068.685	1355.977	1924.311	388.092	1966.733	-38.048
2800	941.548	2102.877	1382.045	2018.330	388.240	2025.237	-37.780
2900	944.045	2135.962	1407.475	2112.612	388.112	2083.690	-37.531
3000	946.318	2168.005	1432.295	2207.132	387.749	2142.178	-37.298
3100	948.393	2199.069	1456.531	2301.869	387.078	2200.608	-37.079
3200	950.290	2229.210	1480.209	2396.804	386.140	2259.135	-36.876
3300	952.030	2258.479	1503.351	2491.922	384.917	2317.733	-36.686
3400	953.629	2286.924	1525.981	2587.206	383.383	2376.290	-36.506
3500	955.102	2314.589	1548.119	2682.643	381.543	2434.878	-36.338
3600	956.461	2341.514	1569.786	2778.222	379.420	2493.609	-36.181
3700	957.718	2367.738	1590.999	2873.932	376.981	2552.416	-36.033
3800	958.883	2393.294	1611.777	2969.763	374.205	2611.239	-35.893
3900	959.963	2418.216	1632.137	3065.706	371.129	2670.087	-35.761
4000	960.968	2442.533	1652.094	3161.753	367.738	2729.152	-35.638
4100	961.904	2466.273	1671.664	3257.897	363.999	2788.235	-35.522
4200	962.776	2489.463	1690.860	3354.132	359.939	2847.405	-35.412
4300	963.591	2512.127	1709.697	3450.451	355.544	2906.590	-35.307
4400	964.354	2534.289	1728.187	3546.848	350.822	2965.968	-35.210
4500	965.068	2555.969	1746.342	3643.320	345.789	3025.509	-35.118
4600	965.738	2577.187	1764.174	3739.860	340.393	3085.176	-35.033
4700	966.367	2597.963	1781.694	3836.466	334.651	3144.855	-34.950
4800	966.959	2618.315	1798.912	3933.132	328.605	3204.760	-34.874
4900	967.516	2638.259	1815.839	4029.857	322.185	3264.666	-34.801
5000	968.041	2657.810	1832.484	4126.635	315.480	3324.882	-34.734

3.274. Anthra[2,1,9,8-*opqra*]naphthacene



Other names: Benzo[*b*]anthanthrene

Formula: C₂₆H₁₄

Mass: 326.389 g/mol

CAS Number: 92586-98-6

Point Group: C_s

Length: 15.30 Å

Width: 9.553 Å

Breadth: 3.885 Å

L/B Ratio: 1.601

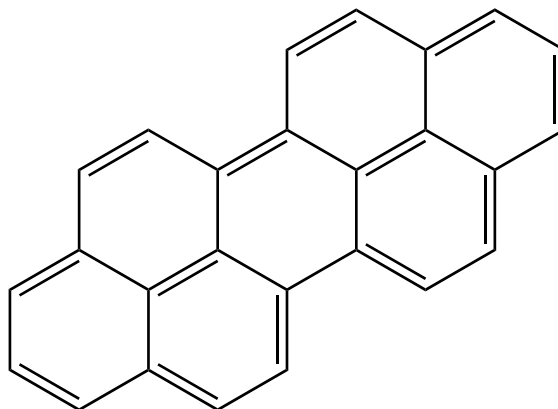
Cartesian coordinates:

C	5.7046	-0.8811	0.0000	C	-5.4784	-0.8952	0.0000	H	5.1030	2.4817	0.0000
C	5.9557	0.5148	0.0000	C	-4.4542	-1.8084	0.0000	H	4.2103	-2.4312	0.0000
C	4.9184	1.4014	0.0000	C	-2.8330	0.0148	0.0000	H	2.7112	2.9298	0.0000
C	4.4234	-1.3512	0.0000	C	-3.1039	-1.3726	0.0000	H	0.3078	3.4029	0.0000
C	3.3157	-0.4539	0.0000	C	-2.0295	-2.2945	0.0000	H	-2.1045	3.8785	0.0000
C	3.5680	0.9388	0.0000	C	-1.4898	0.4718	0.0000	H	-4.4438	3.0664	0.0000
C	2.4974	1.8537	0.0000	C	-0.4386	-0.4514	0.0000	H	-6.0494	1.1965	0.0000
C	1.1846	1.4063	0.0000	C	-0.7211	-1.8522	0.0000	H	-6.5195	-1.2351	0.0000
C	0.0847	2.3287	0.0000	C	0.3897	-2.7733	0.0000	H	-4.6642	-2.8840	0.0000
C	-1.2073	1.8862	0.0000	C	1.6654	-2.3277	0.0000	H	-2.2496	-3.3692	0.0000
C	-2.3298	2.8056	0.0000	C	1.9737	-0.9198	0.0000	H	0.1670	-3.8465	0.0000
C	-3.6020	2.3644	0.0000	C	0.9188	0.0043	0.0000	H	2.5160	-3.0270	0.0000
C	-3.9115	0.9482	0.0000	H	6.5528	-1.5733	0.0000				
C	-5.2133	0.4881	0.0000	H	6.9923	0.8673	0.0000				

Table 3.274: Table of thermodynamic data as a function of temperature for Anthra[2,1,9,8-*opqra*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-46.244	415.518	415.518	∞
100	97.376	334.408	736.743	-40.233	439.326	478.870	-250.131
200	201.505	432.122	559.827	-25.541	426.685	523.463	-136.712
250	261.281	483.469	539.390	-13.980	420.778	548.341	-114.567
298.15	319.228	534.459	534.459	0.000	415.518	573.400	-100.455
300	321.425	536.441	534.465	0.593	415.323	574.378	-100.006
350	379.140	590.368	538.593	18.121	410.463	601.283	-89.735
400	432.659	644.542	548.451	38.436	406.227	628.830	-82.115
450	481.172	698.353	562.123	61.303	402.539	656.881	-76.247
500	524.568	751.340	578.404	86.468	399.322	685.337	-71.595
600	597.382	853.679	615.829	142.710	394.033	743.063	-64.688
700	654.946	950.259	656.778	205.436	390.095	801.570	-59.813
800	701.043	1040.834	699.186	273.318	387.360	860.543	-56.187
900	738.528	1125.642	741.910	345.359	385.673	919.787	-53.382
1000	769.419	1205.103	784.299	420.805	384.892	979.183	-51.146
1100	795.155	1279.680	825.979	499.071	384.842	1038.629	-49.319
1200	816.785	1349.822	866.739	579.699	385.398	1098.035	-47.795
1300	835.100	1415.943	906.467	662.318	386.396	1157.386	-46.503
1400	850.710	1478.416	945.110	746.629	387.719	1216.651	-45.393
1500	864.095	1537.577	982.653	832.386	389.296	1275.815	-44.427
1600	875.636	1593.722	1019.106	919.387	391.009	1334.858	-43.578
1700	885.638	1647.115	1054.490	1007.462	392.795	1393.771	-42.824
1800	894.352	1697.989	1088.838	1096.471	394.584	1452.637	-42.154
1900	901.978	1746.552	1122.186	1186.296	396.351	1511.355	-41.549
2000	908.682	1792.992	1154.574	1276.836	398.047	1570.007	-41.004
2100	914.602	1837.473	1186.041	1368.006	399.601	1628.563	-40.507
2200	919.850	1880.144	1216.628	1459.734	401.014	1687.051	-40.055
2300	924.522	1921.138	1246.374	1551.957	402.282	1745.478	-39.640
2400	928.695	1960.575	1275.316	1644.622	403.340	1803.807	-39.258
2500	932.436	1998.563	1303.491	1737.682	404.200	1862.204	-38.908
2600	935.801	2035.201	1330.933	1831.097	404.828	1920.460	-38.582
2700	938.838	2070.576	1357.676	1924.831	405.231	1978.766	-38.281
2800	941.587	2104.770	1383.750	2018.855	405.383	2037.081	-38.001
2900	944.081	2137.856	1409.187	2113.140	405.259	2095.345	-37.740
3000	946.352	2169.900	1434.013	2207.663	404.899	2153.643	-37.497
3100	948.424	2200.965	1458.254	2302.404	404.232	2211.884	-37.269
3200	950.320	2231.107	1481.937	2397.342	403.296	2270.221	-37.057
3300	952.058	2260.377	1505.085	2492.463	402.076	2328.630	-36.858
3400	953.656	2288.823	1527.720	2587.749	400.545	2386.996	-36.671
3500	955.127	2316.488	1549.863	2683.189	398.708	2445.395	-36.495
3600	956.485	2343.414	1571.534	2778.771	396.587	2503.935	-36.330
3700	957.740	2369.638	1592.751	2874.483	394.151	2562.553	-36.176
3800	958.904	2395.195	1613.533	2970.316	391.377	2621.185	-36.030
3900	959.983	2420.117	1633.897	3066.261	388.303	2679.843	-35.892
4000	960.987	2444.435	1653.857	3162.310	384.914	2738.718	-35.763
4100	961.922	2468.176	1673.430	3258.456	381.177	2797.611	-35.641
4200	962.794	2491.366	1692.630	3354.692	377.118	2856.591	-35.526
4300	963.608	2514.031	1711.470	3451.013	372.725	2915.585	-35.417
4400	964.370	2536.193	1729.963	3547.412	368.005	2974.773	-35.314
4500	965.083	2557.873	1748.121	3643.885	362.973	3034.124	-35.218
4600	965.752	2579.092	1765.955	3740.427	357.579	3093.600	-35.128
4700	966.381	2599.868	1783.478	3837.034	351.838	3153.088	-35.042
4800	966.972	2620.220	1800.699	3933.702	345.793	3212.803	-34.962
4900	967.529	2640.164	1817.628	4030.428	339.374	3272.518	-34.885
5000	968.053	2659.716	1834.275	4127.207	332.671	3332.544	-34.814

3.275. Dibenzo[*cd,lm*]perylene



Other names: Peropyrene
Formula: $C_{26}H_{14}$
Mass: 326.389 g/mol
CAS Number: 188-96-5
Point Group: D_{2h}

Length: 15.86 Å
Width: 9.201 Å
Breadth: 3.884 Å
L/B Ratio: 1.724

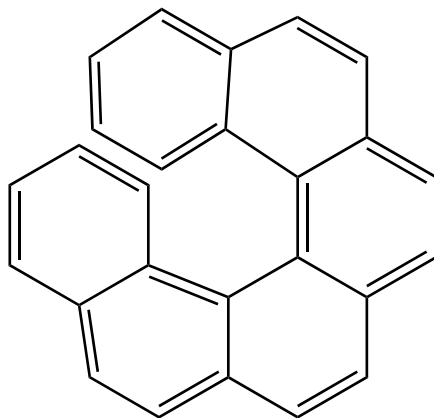
Cartesian coordinates:

C	4.9464	-1.2153	0.0000	C	-1.4556	2.4581	0.0000	H	5.5035	2.1450	0.0000
C	5.6364	-0.0093	0.0000	C	-2.8077	2.4612	0.0000	H	3.3819	3.3904	0.0000
C	4.9503	1.1990	0.0000	C	-3.5482	1.2271	0.0000	H	0.8967	3.3970	0.0000
C	3.5522	1.2154	0.0000	C	-4.9463	1.2153	0.0000	H	0.8854	-3.3998	0.0000
C	2.8158	2.4519	0.0000	C	-5.6364	0.0093	0.0000	H	3.3707	-3.4015	0.0000
C	1.4637	2.4533	0.0000	C	-4.9504	-1.1990	0.0000	H	-0.8855	3.3999	0.0000
C	0.7065	1.2282	0.0000	C	-2.8384	0.0046	0.0000	H	-3.3707	3.4015	0.0000
C	1.4030	-0.0023	0.0000	C	-3.5522	-1.2155	0.0000	H	-5.4964	2.1631	0.0000
C	0.7025	-1.2305	0.0000	C	-2.8158	-2.4519	0.0000	H	-6.7315	0.0112	0.0000
C	1.4556	-2.4580	0.0000	C	-1.4636	-2.4532	0.0000	H	-5.5035	-2.1451	0.0000
C	2.8077	-2.4612	0.0000	C	-0.7065	-1.2281	0.0000	H	-3.3818	-3.3905	0.0000
C	3.5482	-1.2271	0.0000	C	-1.4031	0.0023	0.0000	H	-0.8965	-3.3969	0.0000
C	2.8384	-0.0047	0.0000	H	5.4963	-2.1632	0.0000				
C	-0.7024	1.2305	0.0000	H	6.7315	-0.0110	0.0000				

Table 3.275: Table of thermodynamic data as a function of temperature for Dibenzo[*cd,lm*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-46.205	395.472	395.472	∞
100	97.224	323.607	725.349	-40.174	419.340	459.963	-240.255
200	201.147	421.117	548.680	-25.513	406.668	505.648	-132.059
250	260.985	472.390	528.263	-13.968	400.744	531.078	-110.960
298.15	319.032	523.336	523.336	0.000	395.472	556.671	-97.524
300	321.233	525.316	523.342	0.592	395.278	557.670	-97.097
350	379.063	579.222	527.467	18.114	390.411	585.131	-87.324
400	432.683	633.393	537.323	38.428	386.173	613.236	-80.079
450	481.274	687.212	550.993	61.298	382.489	641.844	-74.502
500	524.722	740.212	567.273	86.469	379.278	670.857	-70.083
600	597.576	842.584	604.702	142.729	374.007	729.694	-63.524
700	655.127	939.193	645.658	205.475	370.088	789.309	-58.898
800	701.190	1029.790	688.074	273.373	367.369	849.387	-55.458
900	738.634	1114.614	730.806	345.426	365.695	909.735	-52.799
1000	769.489	1194.084	773.203	420.881	364.923	970.233	-50.679
1100	795.194	1268.666	814.891	499.153	364.878	1030.781	-48.947
1200	816.800	1338.810	855.657	579.783	365.437	1091.288	-47.502
1300	835.097	1404.931	895.390	662.403	366.435	1151.740	-46.277
1400	850.694	1467.404	934.038	746.713	367.757	1212.106	-45.223
1500	864.070	1526.564	971.585	832.468	369.332	1272.371	-44.307
1600	875.604	1582.707	1008.041	919.465	371.043	1332.517	-43.501
1700	885.602	1636.097	1043.428	1007.537	372.825	1392.530	-42.786
1800	894.313	1686.969	1077.778	1096.543	374.610	1452.499	-42.150
1900	901.937	1735.531	1111.129	1186.364	376.373	1512.319	-41.576
2000	908.641	1781.968	1143.518	1276.900	378.065	1572.073	-41.057
2100	914.561	1826.447	1174.987	1368.066	379.615	1631.732	-40.586
2200	919.810	1869.116	1205.575	1459.790	381.024	1691.322	-40.156
2300	924.483	1910.108	1235.322	1552.009	382.288	1750.852	-39.762
2400	928.657	1949.544	1264.265	1644.670	383.342	1810.284	-39.399
2500	932.399	1987.531	1292.440	1737.726	384.198	1869.784	-39.066
2600	935.766	2024.167	1319.883	1831.137	384.823	1929.144	-38.756
2700	938.804	2059.541	1346.627	1924.868	385.222	1988.553	-38.470
2800	941.553	2093.733	1372.702	2018.888	385.371	2047.971	-38.205
2900	944.049	2126.818	1398.138	2113.170	385.244	2107.339	-37.956
3000	946.321	2158.861	1422.965	2207.691	384.881	2166.741	-37.726
3100	948.395	2189.926	1447.207	2302.428	384.210	2226.086	-37.509
3200	950.292	2220.066	1470.890	2397.364	383.272	2285.527	-37.307
3300	952.031	2249.335	1494.038	2492.481	382.049	2345.040	-37.118
3400	953.630	2277.780	1516.673	2587.765	380.515	2404.511	-36.940
3500	955.102	2305.445	1538.816	2683.203	378.676	2464.014	-36.773
3600	956.461	2332.371	1560.487	2778.782	376.552	2523.658	-36.617
3700	957.717	2358.594	1581.704	2874.491	374.114	2583.380	-36.470
3800	958.882	2384.150	1602.487	2970.322	371.337	2643.117	-36.331
3900	959.962	2409.072	1622.850	3066.265	368.261	2702.880	-36.200
4000	960.967	2433.389	1642.811	3162.312	364.870	2762.859	-36.078
4100	961.902	2457.129	1662.384	3258.456	361.131	2822.857	-35.963
4200	962.775	2480.319	1681.583	3354.690	357.071	2882.941	-35.854
4300	963.590	2502.983	1700.423	3451.009	352.675	2943.041	-35.750
4400	964.352	2525.145	1718.916	3547.407	347.954	3003.333	-35.653
4500	965.066	2546.825	1737.074	3643.878	342.920	3063.788	-35.563
4600	965.736	2568.043	1754.909	3740.418	337.525	3124.370	-35.478
4700	966.365	2588.819	1772.431	3837.024	331.782	3184.963	-35.396
4800	966.957	2609.171	1789.652	3933.690	325.735	3245.783	-35.321
4900	967.514	2629.115	1806.581	4030.414	319.315	3306.602	-35.248
5000	968.039	2648.666	1823.228	4127.192	312.610	3367.734	-35.182

3.276. Phenanthro[3,4-*c*]phenanthrene



Other names: [6] Helicene
Hexahelicene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 187-83-7

Point Group: C₂

Length: 11.50 Å

Width: 11.12 Å

Breadth: 7.670 Å

L/B Ratio: 1.034

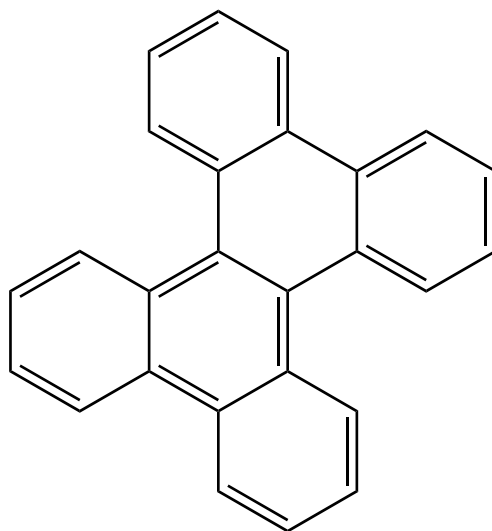
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C	-3.0980	-2.4442	-0.7612	C	1.1382	3.5275	-0.4726	H	-0.3496	-2.8663	-2.7023
C	-0.7120	-1.1746	-1.4348	C	2.2480	2.8538	-0.8799	H	-2.4463	-4.0312	-2.0539
C	-1.0276	-2.3946	-1.9834	C	1.2831	0.7457	-0.0773	H	-4.7045	-1.0289	0.8450
C	-2.2201	-3.0488	-1.6272	C	2.3514	1.4515	-0.6471	H	-4.3487	1.3446	1.5058
C	-1.5724	-0.5487	-0.5013	C	3.5811	0.7866	-0.9555	H	-3.0935	3.3831	1.3316
C	-2.8024	-1.1746	-0.2133	C	3.7811	-0.5017	-0.5834	H	-1.0826	4.6211	0.5322
C	-3.7808	-0.4997	0.5848	C	1.5720	-0.5497	0.5012	H	1.0847	4.6204	-0.5327
C	-3.5799	0.7883	0.9571	C	2.8017	-1.1763	0.2135	H	3.0964	3.3810	-1.3307
C	-1.2825	0.7465	0.0771	C	3.0962	-2.4464	0.7611	H	4.3510	1.3423	-1.5032
C	-2.3501	1.4529	0.6478	C	2.2175	-3.0507	1.6264	H	4.7049	-1.0309	-0.8432
C	-2.2459	2.8551	0.8801	C	1.0253	-2.3958	1.9823	H	4.0410	-2.9342	0.4953
C	-1.1359	3.5281	0.4718	C	0.7108	-1.1754	1.4342	H	2.4426	-4.0336	2.0526
C	0.0005	1.4028	-0.0002	H	-4.0430	-2.9316	-0.4955	H	0.3467	-2.8674	2.7007
C	0.0008	2.8099	-0.0004	H	0.2190	-0.6714	-1.7259	H	-0.2200	-0.6715	1.7249

Table 3.276: Table of thermodynamic data as a function of temperature for Phenanthro[3,4-*c*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.658	481.627	481.627	∞
100	109.021	341.228	770.062	-42.883	508.254	557.188	-291.039
200	214.397	447.241	582.178	-26.987	494.122	611.759	-159.772
250	275.981	501.648	560.605	-14.739	487.506	641.935	-134.122
298.15	336.098	555.409	555.409	0.000	481.627	672.226	-117.769
300	338.380	557.495	555.416	0.624	481.411	673.407	-117.248
350	398.400	614.210	559.758	19.058	476.008	705.846	-105.340
400	454.041	671.097	570.121	40.390	471.331	738.999	-96.501
450	504.418	727.537	584.483	64.374	467.299	772.704	-89.691
500	549.426	783.058	601.574	90.742	463.823	806.848	-84.289
600	624.882	890.174	640.827	149.608	458.229	876.009	-76.262
700	684.596	991.158	683.737	215.195	454.214	945.983	-70.589
800	732.564	1085.817	728.146	286.137	451.586	1016.420	-66.364
900	771.737	1174.437	772.864	361.415	450.162	1087.108	-63.093
1000	804.168	1257.478	817.218	440.260	449.777	1157.909	-60.482
1100	831.305	1335.434	860.822	522.073	450.234	1228.716	-58.346
1200	854.203	1408.776	903.459	606.380	451.391	1299.431	-56.562
1300	873.660	1477.938	945.015	692.799	453.068	1370.039	-55.048
1400	890.293	1543.307	985.437	781.018	455.135	1440.507	-53.745
1500	904.592	1605.231	1024.711	870.780	457.509	1510.817	-52.610
1600	916.948	1664.016	1062.846	961.872	460.063	1580.953	-51.612
1700	927.678	1719.935	1099.867	1054.115	462.722	1650.902	-50.725
1800	937.040	1773.231	1135.807	1147.362	465.415	1720.755	-49.934
1900	945.245	1824.118	1170.705	1241.485	468.108	1790.408	-49.221
2000	952.468	1872.791	1204.602	1336.378	470.747	1859.946	-48.576
2100	958.852	1919.419	1237.538	1431.950	473.257	1929.340	-47.989
2200	964.517	1964.158	1269.556	1528.124	475.637	1998.622	-47.452
2300	969.564	2007.146	1300.697	1624.833	477.880	2067.796	-46.960
2400	974.076	2048.508	1331.000	1722.019	479.918	2136.831	-46.506
2500	978.123	2088.355	1360.502	1819.633	481.762	2205.895	-46.089
2600	981.766	2126.790	1389.240	1917.630	483.376	2274.776	-45.700
2700	985.054	2163.905	1417.248	2015.974	484.763	2343.668	-45.340
2800	988.032	2199.783	1444.558	2114.631	485.900	2412.537	-45.005
2900	990.737	2234.503	1471.202	2213.572	486.757	2481.316	-44.692
3000	993.199	2268.132	1497.209	2312.770	487.375	2550.096	-44.400
3100	995.447	2300.736	1522.606	2412.204	487.681	2618.787	-44.125
3200	997.504	2332.374	1547.419	2511.853	487.714	2687.543	-43.869
3300	999.390	2363.098	1571.674	2611.699	487.456	2756.339	-43.628
3400	1001.125	2392.959	1595.392	2711.726	486.881	2825.066	-43.401
3500	1002.722	2422.002	1618.596	2811.920	485.993	2893.797	-43.187
3600	1004.197	2450.271	1641.308	2912.267	484.812	2962.639	-42.986
3700	1005.562	2477.803	1663.545	3012.755	483.309	3031.538	-42.797
3800	1006.826	2504.637	1685.328	3113.376	481.457	3100.421	-42.617
3900	1007.999	2530.805	1706.672	3214.118	479.297	3169.310	-42.447
4000	1009.090	2556.339	1727.596	3314.973	476.812	3238.390	-42.288
4100	1010.106	2581.269	1748.115	3415.933	473.968	3307.466	-42.137
4200	1011.054	2605.622	1768.243	3516.992	470.793	3376.606	-41.993
4300	1011.939	2629.423	1787.994	3618.142	467.271	3445.740	-41.857
4400	1012.768	2652.696	1807.383	3719.377	463.413	3515.049	-41.728
4500	1013.544	2675.465	1826.422	3820.693	459.231	3584.504	-41.607
4600	1014.272	2697.750	1845.122	3922.085	454.676	3654.061	-41.492
4700	1014.956	2719.570	1863.496	4023.546	449.761	3723.612	-41.382
4800	1015.599	2740.945	1881.555	4125.074	444.534	3793.373	-41.279
4900	1016.204	2761.892	1899.308	4226.665	438.920	3863.117	-41.180
5000	1016.775	2782.428	1916.765	4328.314	433.011	3933.160	-41.089

3.277. Dibenzo[*g,p*]chrysene



Other names: Dibenzo[*a,c*]triphenylene
 1,2:3,4:5,6:7,8-Tetrabenzonaphthalene
 Biphenylenephenanthrene
 Difluorenylene
 9,10-Diphenylenephenanthrene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 191-68-4
Point Group: C_{2h}

Length: 13.82 Å
Width: 12.84 Å
Breadth: 4.699 Å
L/B Ratio: 1.076

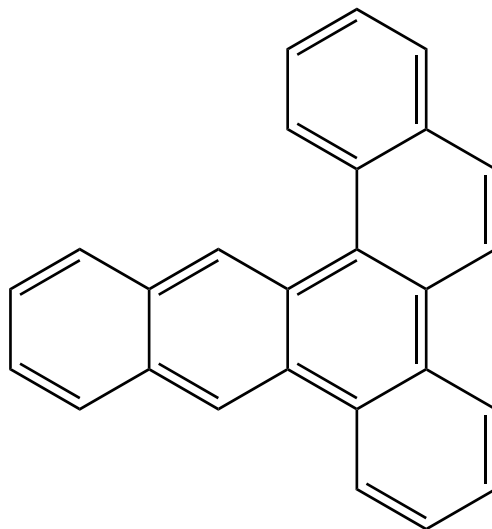
Cartesian coordinates:

C	2.5753	-3.4420	0.3911	C	-1.2636	-1.4128	-0.0850	H	4.5934	-0.8766	-0.5608
C	3.7345	-2.7792	-0.0296	C	-2.4649	-0.7280	0.1758	H	0.4823	-3.3098	0.7887
C	3.6808	-1.4284	-0.2885	C	-3.6747	-1.4441	0.2886	H	4.5896	0.8966	-0.5602
C	1.3749	-2.7676	0.4486	C	-3.7226	-2.7951	0.0297	H	4.6629	3.3476	-0.1210
C	1.2696	-1.4075	0.0849	C	-2.5606	-3.4530	-0.3912	H	2.6064	4.5097	0.6753
C	2.4680	-0.7175	-0.1758	C	-1.3631	-2.7734	-0.4487	H	0.4681	3.3116	0.7895
C	1.2635	1.4128	0.0853	C	-2.4680	0.7176	0.1756	H	-4.5895	-0.8961	0.5609
C	2.4649	0.7281	-0.1755	C	-1.2695	1.4074	-0.0854	H	-4.6630	-3.3475	0.1225
C	3.6746	1.4443	-0.2878	C	-1.3747	2.7673	-0.4496	H	-2.6067	-4.5099	-0.6737
C	3.7225	2.7952	-0.0284	C	-2.5751	3.4419	-0.3924	H	-0.4682	-3.3116	-0.7890
C	2.5604	3.4529	0.3924	C	-3.7344	2.7793	0.0286	H	-0.4822	3.3095	-0.7898
C	1.3629	2.7732	0.4494	C	-3.6807	1.4286	0.2880	H	-2.6257	4.4985	-0.6753
C	0.0015	-0.6942	-0.0000	H	2.6260	-4.4987	0.6737	H	-4.6771	3.3277	0.1212
C	-0.0015	0.6941	-0.0000	H	4.6773	-3.3275	-0.1224	H	-4.5933	0.8769	0.5604

Table 3.277: Table of thermodynamic data as a function of temperature for Dibenzo[*g,p*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.457	489.689	489.689	∞
100	109.330	342.461	769.626	-42.717	516.482	565.293	-295.273
200	213.475	448.504	582.624	-26.824	502.347	619.732	-161.854
250	274.239	502.609	561.185	-14.644	495.663	649.851	-135.776
298.15	333.942	556.024	556.024	0.000	489.689	680.104	-119.149
300	336.216	558.096	556.030	0.620	489.469	681.284	-118.620
350	396.117	614.466	560.345	18.942	483.953	713.702	-106.512
400	451.814	671.050	570.648	40.161	479.164	746.850	-97.527
450	502.326	727.235	584.931	64.037	475.023	780.564	-90.604
500	547.493	782.544	601.936	90.304	471.447	814.729	-85.112
600	623.234	889.333	641.015	148.991	465.674	883.958	-76.954
700	683.154	990.080	683.760	214.424	461.505	954.029	-71.189
800	731.264	1084.556	728.019	285.229	458.740	1024.583	-66.897
900	770.539	1173.029	772.603	360.383	457.192	1095.404	-63.574
1000	803.053	1255.949	816.836	439.113	456.691	1166.353	-60.923
1100	830.262	1333.801	860.331	520.818	457.040	1237.317	-58.754
1200	853.227	1407.056	902.869	605.024	458.096	1308.201	-56.943
1300	872.747	1476.142	944.335	691.348	459.679	1378.985	-55.407
1400	889.441	1541.446	984.675	779.479	461.658	1449.635	-54.085
1500	903.797	1603.313	1023.874	869.159	463.949	1520.134	-52.935
1600	916.206	1662.048	1061.940	960.174	466.426	1590.464	-51.922
1700	926.986	1717.924	1098.897	1052.346	469.014	1660.612	-51.023
1800	936.395	1771.181	1134.779	1145.525	471.640	1730.669	-50.222
1900	944.643	1822.035	1169.622	1239.586	474.271	1800.529	-49.499
2000	951.906	1870.678	1203.467	1334.421	476.852	1870.276	-48.846
2100	958.327	1917.280	1236.357	1429.939	479.308	1939.883	-48.251
2200	964.026	1961.996	1268.331	1526.062	481.637	2009.380	-47.708
2300	969.104	2004.962	1299.430	1622.724	483.832	2078.771	-47.209
2400	973.644	2046.305	1329.694	1719.865	485.826	2148.026	-46.750
2500	977.718	2086.135	1359.160	1817.437	487.628	2217.310	-46.327
2600	981.385	2124.554	1387.864	1915.395	489.202	2286.414	-45.934
2700	984.696	2161.655	1415.840	2013.702	490.553	2355.531	-45.570
2800	987.695	2197.522	1443.120	2112.324	491.655	2424.625	-45.231
2900	990.418	2232.229	1469.736	2211.232	492.479	2493.631	-44.914
3000	992.898	2265.848	1495.715	2310.400	493.066	2562.639	-44.619
3100	995.162	2298.443	1521.087	2409.804	493.343	2631.559	-44.341
3200	997.234	2330.071	1545.876	2509.426	493.348	2700.545	-44.081
3300	999.135	2360.787	1570.107	2609.246	493.064	2769.572	-43.838
3400	1000.882	2390.641	1593.803	2709.248	492.464	2838.530	-43.608
3500	1002.492	2419.677	1616.987	2809.417	491.552	2907.492	-43.391
3600	1003.978	2447.940	1639.678	2909.742	490.348	2976.568	-43.188
3700	1005.353	2475.466	1661.896	3010.209	488.824	3045.700	-42.997
3800	1006.626	2502.295	1683.661	3110.809	486.952	3114.817	-42.815
3900	1007.809	2528.458	1704.988	3211.531	484.772	3183.940	-42.643
4000	1008.908	2553.987	1725.895	3312.368	482.269	3253.256	-42.482
4100	1009.932	2578.913	1746.398	3413.311	479.407	3322.566	-42.329
4200	1010.888	2603.261	1766.511	3514.352	476.215	3391.943	-42.184
4300	1011.780	2627.058	1786.248	3615.486	472.677	3461.313	-42.046
4400	1012.615	2650.328	1805.622	3716.706	468.803	3530.858	-41.916
4500	1013.397	2673.093	1824.647	3818.007	464.606	3600.550	-41.793
4600	1014.131	2695.375	1843.335	3919.384	460.037	3670.345	-41.677
4700	1014.821	2717.193	1861.696	4020.832	455.109	3740.133	-41.566
4800	1015.469	2738.565	1879.743	4122.347	449.868	3810.132	-41.462
4900	1016.079	2759.509	1897.484	4223.925	444.241	3880.114	-41.362
5000	1016.655	2780.043	1914.931	4325.562	438.320	3950.396	-41.269

3.278. Naphtho[2,3-*g*]chrysene



Other names: Dibenz[*a,n*]triphenylene
Dibenzo[*a,f*]tetraphene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 196-64-5
Point Group: C₁

Length: 13.96 Å
Width: 12.53 Å
Breadth: 5.067 Å
L/B Ratio: 1.114

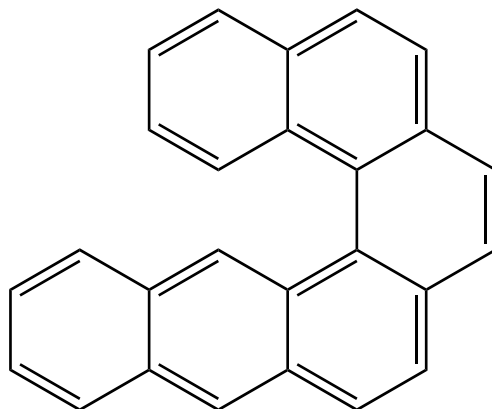
Cartesian coordinates:

C	4.6019	-2.5524	0.3794	C	-1.0243	4.7174	-0.0528	H	5.1417	0.7404	-0.3722
C	5.2977	-1.3539	0.0736	C	-1.6949	3.5323	0.1779	H	2.6945	-3.4841	0.6931
C	4.6145	-0.1914	-0.1394	C	-1.1066	-0.1828	0.0542	H	2.9926	1.9602	-0.4041
C	3.2390	-2.5629	0.4571	C	-1.7486	1.0383	0.2481	H	0.5790	-2.3009	0.5044
C	2.4975	-1.3660	0.2293	C	-3.1390	1.0754	0.5559	H	2.0898	3.4744	-0.6499
C	3.1913	-0.1720	-0.0590	C	-3.8829	-0.0625	0.5915	H	0.8657	5.6389	-0.5595
C	2.4540	1.0151	-0.2275	C	-1.9213	-1.3628	-0.1049	H	-1.5579	5.6718	0.0041
C	1.0888	-1.3535	0.2755	C	-3.2965	-1.3015	0.2107	H	-2.7687	3.5494	0.4170
C	0.3563	-0.2017	0.0363	C	-4.1129	-2.4571	0.1058	H	-3.6026	2.0484	0.7782
C	1.0715	1.0216	-0.1498	C	-3.5950	-3.6333	-0.3666	H	-4.9417	-0.0378	0.8732
C	-1.0277	2.2958	0.1048	C	-2.2448	-3.6863	-0.7677	H	-5.1668	-2.3880	0.3991
C	0.3470	2.2834	-0.1757	C	-1.4367	-2.5869	-0.6394	H	-4.2194	-4.5284	-0.4506
C	1.0134	3.4969	-0.4213	H	5.1777	-3.4677	0.5513	H	-1.8491	-4.6164	-1.1892
C	0.3376	4.6998	-0.3655	H	6.3907	-1.3784	0.0135	H	-0.3908	-2.6536	-0.9692

Table 3.278: Table of thermodynamic data as a function of temperature for Naphtho[2,3-g]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-50.008	451.254	451.254	∞
100	111.261	354.896	785.190	-43.029	477.735	525.302	-274.384
200	215.008	462.043	596.942	-26.980	463.756	578.433	-151.068
250	275.848	516.500	575.384	-14.721	457.151	607.867	-127.004
298.15	335.503	570.196	570.196	0.000	451.254	637.444	-111.675
300	337.772	572.278	570.202	0.623	451.037	638.598	-111.187
350	397.515	628.877	574.536	19.019	445.595	670.301	-100.035
400	453.014	685.635	584.878	40.303	440.871	702.723	-91.764
450	503.332	741.950	599.208	64.234	436.786	735.705	-85.397
500	548.333	797.356	616.262	90.547	433.255	769.131	-80.349
600	623.844	904.276	655.433	149.306	427.554	836.872	-72.855
700	683.641	1005.107	698.260	214.793	423.439	905.444	-67.564
800	731.693	1099.643	742.589	285.644	420.720	974.493	-63.627
900	770.942	1188.165	787.233	360.839	419.213	1043.803	-60.579
1000	803.441	1271.126	831.519	439.608	418.752	1113.235	-58.148
1100	830.639	1349.015	875.060	521.351	419.139	1182.680	-56.160
1200	853.593	1422.302	917.640	605.594	420.232	1252.041	-54.499
1300	873.100	1491.417	959.144	691.955	421.851	1321.298	-53.089
1400	889.779	1556.747	999.518	780.120	423.864	1390.420	-51.876
1500	904.119	1618.636	1038.748	869.833	426.188	1459.388	-50.819
1600	916.512	1677.392	1076.843	960.879	428.697	1528.185	-49.889
1700	927.276	1733.286	1113.827	1053.081	431.315	1596.797	-49.063
1800	936.668	1786.559	1149.732	1146.288	433.968	1665.317	-48.325
1900	944.901	1837.428	1184.598	1240.376	436.626	1733.638	-47.660
2000	952.149	1886.083	1218.465	1335.236	439.232	1801.846	-47.058
2100	958.556	1932.697	1251.374	1430.778	441.712	1869.912	-46.511
2200	964.242	1977.423	1283.367	1526.923	444.063	1937.866	-46.010
2300	969.308	2020.399	1314.483	1623.605	446.279	2005.714	-45.550
2400	973.836	2061.750	1344.763	1720.767	448.293	2073.425	-45.126
2500	977.899	2101.587	1374.245	1818.357	450.113	2141.165	-44.736
2600	981.556	2140.014	1402.963	1916.333	451.705	2208.723	-44.373
2700	984.858	2177.121	1430.952	2014.657	453.073	2276.293	-44.037
2800	987.848	2212.993	1458.245	2113.294	454.190	2343.841	-43.724
2900	990.563	2247.706	1484.872	2212.217	455.029	2411.300	-43.431
3000	993.035	2281.330	1510.864	2311.399	455.631	2478.759	-43.158
3100	995.292	2313.929	1536.246	2410.817	455.921	2546.131	-42.901
3200	997.357	2345.561	1561.045	2510.451	455.939	2613.568	-42.661
3300	999.252	2376.281	1585.286	2610.283	455.667	2681.046	-42.437
3400	1000.993	2406.138	1608.992	2710.296	455.078	2748.454	-42.224
3500	1002.598	2435.177	1632.184	2810.477	454.177	2815.867	-42.024
3600	1004.079	2463.442	1654.884	2910.812	452.983	2883.392	-41.836
3700	1005.449	2490.972	1677.110	3011.289	451.469	2950.974	-41.659
3800	1006.718	2517.803	1698.882	3111.898	449.606	3018.540	-41.492
3900	1007.897	2543.968	1720.217	3212.629	447.435	3086.113	-41.333
4000	1008.992	2569.500	1741.131	3313.475	444.940	3153.877	-41.185
4100	1010.013	2594.427	1761.640	3414.425	442.087	3221.636	-41.043
4200	1010.965	2618.778	1781.760	3515.475	438.903	3289.461	-40.910
4300	1011.854	2642.577	1801.503	3616.616	435.372	3357.280	-40.782
4400	1012.686	2665.848	1820.884	3717.844	431.506	3425.273	-40.662
4500	1013.465	2688.615	1839.915	3819.152	427.316	3493.413	-40.550
4600	1014.197	2710.898	1858.608	3920.535	422.753	3561.655	-40.443
4700	1014.883	2732.717	1876.974	4021.990	417.831	3629.892	-40.341
4800	1015.529	2754.091	1895.026	4123.510	412.596	3698.338	-40.245
4900	1016.138	2775.036	1912.772	4225.094	406.976	3766.767	-40.153
5000	1016.711	2795.571	1930.224	4326.737	401.061	3835.496	-40.068

3.279. Phenanthro[4,3-*a*]anthracene



Other names: Naphtho[1,2-*a*]tetraphene
Benzo[*b*]pentahelicene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 58029-40-6
Point Group: C₁

Length: 13.69 Å
Width: 11.79 Å
Breadth: 6.299 Å
L/B Ratio: 1.162

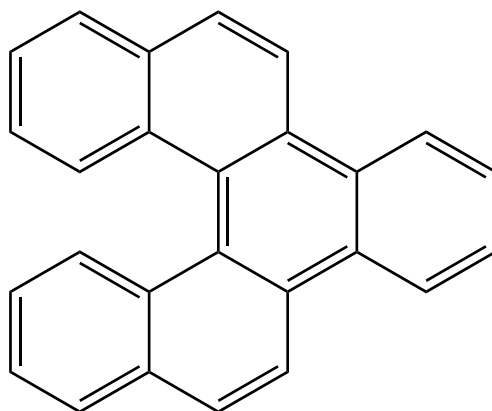
Cartesian coordinates:

C	-4.2762	-2.1505	1.0412	C	2.3115	3.1472	0.2143	H	-5.5432	0.6399	-0.4793
C	-5.2233	-1.2529	0.4776	C	3.2590	2.2771	0.6742	H	-2.2123	-2.5227	1.4916
C	-4.8205	-0.0603	-0.0454	C	1.8174	0.3811	0.0956	H	-3.7348	2.2641	-0.8990
C	-2.9499	-1.8362	1.0602	C	3.0270	0.8791	0.6093	H	0.1043	-0.8371	-1.6590
C	-2.4932	-0.5987	0.5110	C	4.0489	-0.0203	1.0606	H	-1.9817	3.9019	-1.2457
C	-3.4387	0.3015	-0.0351	C	3.9171	-1.3575	0.8907	H	0.3493	4.6403	-0.7860
C	-2.9989	1.5423	-0.5232	C	1.7926	-1.0122	-0.3036	H	2.5128	4.2234	0.1653
C	-1.1276	-0.2670	0.4974	C	2.8126	-1.8774	0.1391	H	4.2192	2.6415	1.0565
C	-0.6803	0.9286	-0.0528	C	2.7908	-3.2432	-0.2229	H	4.9283	0.4022	1.5603
C	-1.6504	1.8731	-0.5021	C	1.8227	-3.7212	-1.0731	H	4.6683	-2.0573	1.2739
C	-1.2332	3.2095	-0.8440	C	0.8625	-2.8422	-1.6024	H	3.5674	-3.9103	0.1684
C	0.0362	3.6046	-0.6102	C	0.8486	-1.5191	-1.2276	H	1.8042	-4.7780	-1.3581
C	0.7279	1.3017	-0.0638	H	-4.6319	-3.0978	1.4594	H	0.1251	-3.2182	-2.3193
C	1.0284	2.6670	-0.1511	H	-6.2807	-1.5368	0.4729	H	-0.4071	-0.9739	0.9325

Table 3.279: Table of thermodynamic data as a function of temperature for Phenanthro[4,3-*a*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.615	471.138	471.138	∞
100	108.733	348.919	777.432	-42.851	497.797	545.962	-285.175
200	214.273	454.816	589.672	-26.971	483.649	599.771	-156.641
250	275.821	509.192	568.111	-14.730	477.026	629.569	-131.539
298.15	335.868	562.919	562.919	0.000	471.138	659.498	-115.539
300	338.147	565.004	562.926	0.623	470.922	660.665	-115.030
350	398.079	621.677	567.265	19.044	465.504	692.730	-103.382
400	453.643	678.515	577.620	40.358	460.810	725.510	-94.740
450	503.963	734.905	591.970	64.321	456.757	758.846	-88.083
500	548.939	790.376	609.047	90.665	453.257	792.623	-82.803
600	624.386	897.401	648.267	149.481	447.613	861.056	-74.960
700	684.135	998.311	691.141	215.019	443.550	930.312	-69.419
800	732.155	1092.912	735.514	285.918	440.878	1000.037	-65.294
900	771.382	1181.487	780.200	361.158	439.416	1070.017	-62.101
1000	803.862	1264.493	824.523	439.970	438.998	1140.115	-59.552
1100	831.042	1342.422	868.099	521.754	439.427	1210.221	-57.467
1200	853.977	1415.743	910.712	606.037	440.559	1280.239	-55.726
1300	873.464	1484.887	952.245	692.435	442.215	1350.152	-54.249
1400	890.123	1550.244	992.647	780.636	444.264	1419.924	-52.977
1500	904.444	1612.156	1031.902	870.382	446.622	1489.542	-51.869
1600	916.817	1670.932	1070.020	961.460	449.162	1558.985	-50.895
1700	927.562	1726.844	1107.026	1053.691	451.809	1628.243	-50.029
1800	936.937	1780.133	1142.952	1146.927	454.491	1697.406	-49.256
1900	945.153	1831.016	1177.837	1241.040	457.174	1766.369	-48.560
2000	952.385	1879.684	1211.721	1335.924	459.805	1835.217	-47.930
2100	958.777	1926.308	1244.647	1431.489	462.307	1903.923	-47.357
2200	964.450	1971.044	1276.655	1527.656	464.680	1972.515	-46.833
2300	969.502	2014.029	1307.787	1624.358	466.916	2041.001	-46.352
2400	974.019	2055.388	1338.081	1721.539	468.949	2109.348	-45.908
2500	978.071	2095.233	1367.575	1819.147	470.787	2177.724	-45.500
2600	981.718	2133.666	1396.305	1917.139	472.395	2245.917	-45.120
2700	985.010	2170.779	1424.306	2015.479	473.779	2314.122	-44.768
2800	987.992	2206.657	1451.610	2114.131	474.911	2382.303	-44.441
2900	990.699	2241.375	1478.248	2213.068	475.764	2450.396	-44.135
3000	993.164	2275.003	1504.249	2312.263	476.379	2518.488	-43.850
3100	995.414	2307.606	1529.640	2411.693	476.681	2586.492	-43.581
3200	997.473	2339.242	1554.448	2511.339	476.711	2654.561	-43.330
3300	999.361	2369.965	1578.698	2611.182	476.450	2722.671	-43.095
3400	1001.098	2399.825	1602.412	2711.206	475.873	2790.711	-42.873
3500	1002.697	2428.868	1625.612	2811.397	474.981	2858.755	-42.664
3600	1004.173	2457.136	1648.319	2911.742	473.798	2926.911	-42.467
3700	1005.539	2484.668	1670.552	3012.228	472.292	2995.123	-42.283
3800	1006.804	2511.501	1692.331	3112.846	470.438	3063.319	-42.107
3900	1007.978	2537.669	1713.672	3213.586	468.276	3131.522	-41.941
4000	1009.071	2563.202	1734.592	3314.439	465.789	3199.916	-41.786
4100	1010.088	2588.131	1755.108	3415.398	462.944	3268.305	-41.638
4200	1011.036	2612.484	1775.233	3516.454	459.766	3336.760	-41.498
4300	1011.923	2636.284	1794.981	3617.603	456.243	3405.207	-41.364
4400	1012.752	2659.558	1814.367	3718.837	452.383	3473.830	-41.239
4500	1013.529	2682.326	1833.403	3820.151	448.199	3542.599	-41.121
4600	1014.257	2704.610	1852.101	3921.541	443.643	3611.470	-41.009
4700	1014.942	2726.430	1870.473	4023.001	438.727	3680.335	-40.901
4800	1015.585	2747.805	1888.528	4124.528	433.498	3749.410	-40.801
4900	1016.191	2768.752	1906.279	4226.117	427.883	3818.467	-40.705
5000	1016.763	2789.288	1923.735	4327.765	421.973	3887.825	-40.615

3.280. Naphtho[1,2-*g*]chrysene



Other names: Benzo[*i*]pentahelicene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 191-67-3

Point Group: C₂

Length: 13.60 Å

Width: 11.71 Å

Breadth: 5.974 Å

L/B Ratio: 1.161

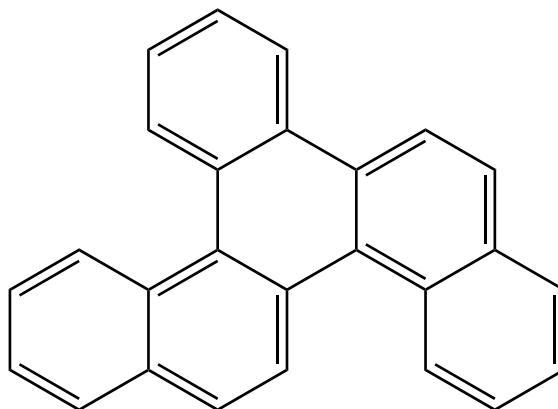
Cartesian coordinates:

C	3.3521	-3.2265	0.7146	C	1.1101	2.9123	0.1932	H	2.2428	0.0809	-1.3456
C	3.3315	-1.9047	1.2020	C	1.1331	1.5590	-0.2014	H	2.2585	-4.7546	-0.3267
C	2.2590	-1.0871	0.9497	C	2.2484	1.1060	-0.9528	H	-2.1330	-3.1698	-1.1631
C	2.2697	-3.7191	0.0322	C	3.3137	1.9323	-1.2068	H	-0.0215	-4.4951	-1.1328
C	1.1361	-2.9012	-0.1991	C	3.3221	3.2559	-0.7235	H	-0.0595	4.4963	1.1289
C	1.1471	-1.5487	0.1987	C	2.2355	3.7405	-0.0422	H	-2.1585	3.1519	1.1660
C	-1.1890	-2.7287	-0.8081	C	-2.4621	-0.6654	-0.2522	H	2.2459	-0.0621	1.3426
C	-0.0445	-3.4604	-0.7728	C	-2.4673	0.6436	0.2588	H	4.1659	1.5697	-1.7910
C	-1.2023	-1.3628	-0.3930	C	-3.7013	1.2647	0.5456	H	4.1917	3.8930	-0.9138
C	-0.0062	-0.7230	-0.0662	C	-4.8906	0.6208	0.2883	H	2.2140	4.7772	0.3126
C	-1.2135	1.3527	0.3950	C	-4.8856	-0.6659	-0.2708	H	-3.6949	2.2796	0.9713
C	-0.0125	0.7235	0.0657	C	-3.6914	-1.2984	-0.5335	H	-5.8438	1.1106	0.5117
C	-0.0740	3.4612	0.7695	H	4.2286	-3.8555	0.9006	H	-5.8351	-1.1650	-0.4898
C	-1.2116	2.7190	0.8087	H	4.1795	-1.5362	1.7886	H	-3.6771	-2.3140	-0.9571

Table 3.280: Table of thermodynamic data as a function of temperature for Naphtho[1,2-g]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-49.791	470.299	470.299	∞
100	110.328	343.328	773.021	-42.969	496.840	545.564	-284.968
200	214.769	450.059	584.937	-26.976	482.806	599.880	-156.669
250	275.820	504.488	563.379	-14.723	476.194	629.913	-131.611
298.15	335.610	558.190	558.190	0.000	470.299	660.069	-115.639
300	337.883	560.273	558.197	0.623	470.082	661.245	-115.131
350	397.717	616.896	562.532	19.027	464.649	693.547	-103.504
400	453.270	673.685	572.879	40.323	459.936	726.568	-94.878
450	503.618	730.032	587.216	64.267	455.865	760.146	-88.234
500	548.627	785.469	604.279	90.595	452.349	794.168	-82.964
600	624.120	892.442	643.471	149.382	446.676	863.095	-75.138
700	683.875	993.312	686.319	214.895	442.587	932.848	-69.609
800	731.881	1087.877	730.668	285.767	439.888	1003.075	-65.493
900	771.086	1176.418	775.331	360.979	438.398	1073.560	-62.307
1000	803.549	1259.393	819.632	439.760	437.949	1144.167	-59.764
1100	830.718	1337.291	863.188	521.513	438.346	1214.785	-57.684
1200	853.649	1410.583	905.781	605.763	439.446	1285.317	-55.947
1300	873.139	1479.702	947.296	692.128	441.069	1355.747	-54.473
1400	889.804	1545.034	987.680	780.296	443.086	1426.040	-53.205
1500	904.134	1606.925	1026.918	870.011	445.412	1496.179	-52.100
1600	916.520	1665.682	1065.020	961.059	447.922	1566.147	-51.128
1700	927.279	1721.576	1102.010	1053.261	450.540	1635.930	-50.265
1800	936.667	1774.849	1137.922	1146.469	453.194	1705.621	-49.495
1900	944.897	1825.717	1172.793	1240.556	455.851	1775.113	-48.800
2000	952.142	1874.372	1206.665	1335.415	458.457	1844.492	-48.172
2100	958.548	1920.986	1239.578	1430.956	460.936	1913.729	-47.600
2200	964.233	1965.711	1271.574	1527.101	463.286	1982.854	-47.078
2300	969.298	2008.687	1302.695	1623.782	465.502	2051.874	-46.599
2400	973.826	2050.037	1332.978	1720.943	467.514	2120.756	-46.156
2500	977.888	2089.875	1362.462	1818.532	469.333	2189.667	-45.750
2600	981.545	2128.301	1391.183	1916.507	470.924	2258.396	-45.371
2700	984.847	2165.407	1419.174	2014.829	472.290	2327.138	-45.020
2800	987.837	2201.279	1446.470	2113.466	473.407	2395.857	-44.694
2900	990.552	2235.991	1473.099	2212.387	474.245	2464.487	-44.389
3000	993.025	2269.615	1499.092	2311.568	474.845	2533.118	-44.105
3100	995.282	2302.214	1524.476	2410.985	475.134	2601.661	-43.837
3200	997.347	2333.846	1549.277	2510.618	475.151	2670.270	-43.587
3300	999.242	2364.565	1573.520	2610.449	474.878	2738.919	-43.353
3400	1000.984	2394.422	1597.227	2710.461	474.289	2807.499	-43.131
3500	1002.589	2423.461	1620.421	2810.641	473.386	2876.084	-42.922
3600	1004.070	2451.726	1643.122	2910.975	472.192	2944.781	-42.727
3700	1005.440	2479.255	1665.350	3011.451	470.677	3013.534	-42.543
3800	1006.710	2506.086	1687.123	3112.060	468.813	3082.272	-42.368
3900	1007.889	2532.251	1708.459	3212.790	466.642	3151.016	-42.202
4000	1008.985	2557.782	1729.374	3313.635	464.146	3219.952	-42.047
4100	1010.005	2582.710	1749.884	3414.585	461.292	3288.883	-41.900
4200	1010.957	2607.060	1770.004	3515.633	458.107	3357.880	-41.760
4300	1011.847	2630.859	1789.748	3616.774	454.575	3426.870	-41.627
4400	1012.679	2654.130	1809.130	3718.001	450.708	3496.035	-41.502
4500	1013.459	2676.897	1828.162	3819.308	446.518	3565.347	-41.385
4600	1014.190	2699.180	1846.855	3920.691	441.954	3634.761	-41.273
4700	1014.877	2720.998	1865.223	4022.145	437.032	3704.169	-41.166
4800	1015.523	2742.372	1883.275	4123.665	431.796	3773.787	-41.066
4900	1016.132	2763.318	1901.022	4225.248	426.176	3843.388	-40.970
5000	1016.705	2783.852	1918.474	4326.890	420.260	3913.289	-40.881

3.281. Dibenzo[*c,p*]chrysene



Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 196-52-1
Point Group: C₁

Length: 13.99 Å
Width: 11.60 Å
Breadth: 5.530 Å
L/B Ratio: 1.205

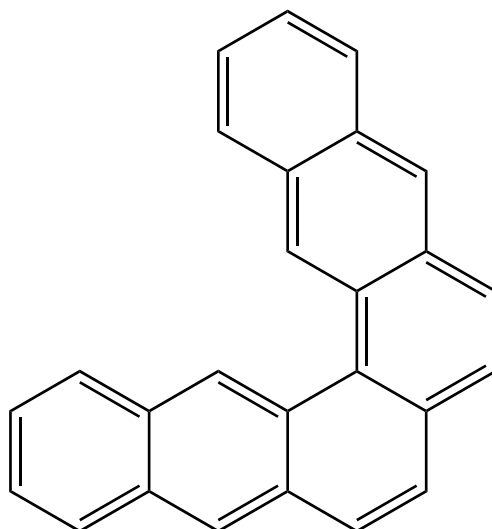
Cartesian coordinates:

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C	4.9843	-1.9775	-0.3878	C	-2.3952	2.2724	0.0689	H	1.6519	-2.6607	-0.3105
C	4.9459	-0.6176	-0.2219	C	-0.0277	-0.6140	0.3425	H	4.6405	2.0221	-0.0168
C	2.5755	-2.0678	-0.2653	C	-1.2254	0.0515	0.0600	H	2.4894	3.2405	0.0081
C	2.4954	-0.6683	-0.0437	C	-1.2679	-2.6007	1.0089	H	0.9984	4.1214	0.1233
C	3.7069	0.0546	-0.0773	C	-0.0951	-1.9231	0.9133	H	-1.1100	5.4133	0.1462
C	3.6888	1.4784	-0.0130	C	-2.4464	-2.0591	0.4161	H	-3.2959	4.2197	0.1524
C	2.5044	2.1406	0.0130	C	-2.4217	-0.7469	-0.0993	H	-3.3720	1.7701	0.0857
C	1.2495	0.0447	0.1362	C	-3.5588	-0.3133	-0.8262	H	-1.3200	-3.5782	1.5013
C	1.2628	1.4367	0.0654	C	-4.6724	-1.1063	-0.9542	H	0.8266	-2.3709	1.3093
C	-1.2118	1.5011	0.0191	C	-4.7144	-2.3805	-0.3587	H	-3.5438	0.6735	-1.3089
C	0.0212	2.1815	0.0629	C	-3.6135	-2.8529	0.3096	H	-5.5365	-0.7534	-1.5269
C	0.0335	3.5937	0.1016	H	3.8118	-3.7853	-0.6027	H	-5.6195	-2.9897	-0.4474
C	-1.1344	4.3193	0.1186	H	5.9383	-2.5021	-0.5008	H	-3.6171	-3.8537	0.7564

Table 3.281: Table of thermodynamic data as a function of temperature for Dibenzo[*c,p*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.764	474.221	474.221	∞
100	110.062	350.957	780.213	-42.926	500.805	548.766	-286.640
200	214.550	457.529	592.302	-26.955	486.748	602.328	-157.309
250	275.603	511.908	570.760	-14.713	480.126	631.989	-132.044
298.15	335.416	565.575	565.575	0.000	474.221	661.788	-115.940
300	337.690	567.657	565.581	0.623	474.003	662.951	-115.428
350	397.563	624.252	569.914	19.018	468.561	694.885	-103.704
400	453.159	681.024	580.256	40.307	463.842	727.538	-95.005
450	503.544	737.360	594.589	64.247	459.766	760.750	-88.304
500	548.583	792.791	611.647	90.572	456.247	794.405	-82.989
600	624.110	899.759	650.831	149.357	450.571	862.600	-75.094
700	683.877	1000.629	693.672	214.869	446.482	931.622	-69.517
800	731.881	1095.194	738.017	285.741	443.784	1001.117	-65.365
900	771.081	1183.735	782.676	360.953	442.294	1070.871	-62.150
1000	803.537	1266.708	826.975	439.733	441.844	1140.746	-59.585
1100	830.699	1344.605	870.528	521.484	442.239	1210.632	-57.487
1200	853.625	1417.896	913.119	605.732	443.337	1280.433	-55.735
1300	873.112	1487.012	954.631	692.095	444.958	1350.132	-54.248
1400	889.775	1552.342	995.013	780.261	446.971	1419.693	-52.968
1500	904.104	1614.231	1034.250	869.972	449.295	1489.102	-51.854
1600	916.490	1672.986	1072.350	961.017	451.801	1558.339	-50.874
1700	927.248	1728.878	1109.339	1053.216	454.417	1627.393	-50.003
1800	936.637	1782.150	1145.249	1146.421	457.067	1696.353	-49.226
1900	944.868	1833.016	1180.119	1240.505	459.721	1765.116	-48.525
2000	952.114	1881.670	1213.989	1335.362	462.324	1833.764	-47.892
2100	958.520	1928.282	1246.901	1430.900	464.800	1902.271	-47.315
2200	964.207	1973.006	1278.896	1527.042	467.148	1970.667	-46.789
2300	969.272	2015.981	1310.015	1623.720	469.361	2038.957	-46.305
2400	973.802	2057.330	1340.297	1720.878	471.371	2107.110	-45.859
2500	977.865	2097.166	1369.780	1818.465	473.188	2175.292	-45.449
2600	981.523	2135.592	1398.500	1916.438	474.776	2243.292	-45.067
2700	984.826	2172.698	1426.491	2014.758	476.141	2311.305	-44.714
2800	987.817	2208.568	1453.785	2113.393	477.255	2379.294	-44.385
2900	990.533	2243.280	1480.414	2212.312	478.091	2447.196	-44.078
3000	993.006	2276.903	1506.406	2311.491	478.690	2515.098	-43.791
3100	995.264	2309.501	1531.789	2410.906	478.977	2582.913	-43.521
3200	997.331	2341.132	1556.589	2510.538	478.992	2650.792	-43.269
3300	999.226	2371.851	1580.831	2610.367	478.718	2718.713	-43.033
3400	1000.969	2401.708	1604.538	2710.378	478.126	2786.565	-42.809
3500	1002.574	2430.747	1627.731	2810.556	477.223	2854.420	-42.599
3600	1004.056	2459.011	1650.431	2910.889	476.027	2922.389	-42.402
3700	1005.427	2486.540	1672.658	3011.364	474.510	2990.414	-42.216
3800	1006.697	2513.370	1694.431	3111.971	472.645	3058.423	-42.040
3900	1007.877	2539.535	1715.766	3212.700	470.473	3126.439	-41.873
4000	1008.973	2565.066	1736.680	3313.543	467.976	3194.647	-41.717
4100	1009.994	2589.993	1757.190	3414.492	465.121	3262.849	-41.568
4200	1010.947	2614.343	1777.310	3515.540	461.934	3331.118	-41.428
4300	1011.837	2638.142	1797.053	3616.680	458.402	3399.380	-41.293
4400	1012.669	2661.413	1816.435	3717.905	454.534	3467.816	-41.167
4500	1013.449	2684.179	1835.466	3819.212	450.342	3536.400	-41.049
4600	1014.181	2706.462	1854.159	3920.594	445.778	3605.086	-40.936
4700	1014.869	2728.281	1872.526	4022.047	440.855	3673.766	-40.828
4800	1015.515	2749.654	1890.578	4123.566	435.619	3742.655	-40.728
4900	1016.124	2770.600	1908.324	4225.148	429.997	3811.528	-40.631
5000	1016.697	2791.134	1925.776	4326.790	424.080	3880.701	-40.541

3.282. Anthra[1,2-*a*]anthracene



Other names: Naphtho[2,3-*a*]tetraphene
Anthraceno-1',2',1,2-anthracene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 195-00-6
Point Group: C₂

Length: 14.79 Å
Width: 11.31 Å
Breadth: 4.984 Å
L/B Ratio: 1.308

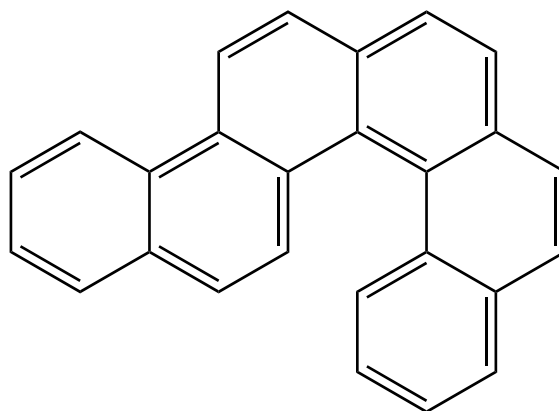
Cartesian coordinates:

C	4.0885	3.1852	-0.5273	C	-1.1955	-3.5715	-0.2762	H	5.9901	0.5410	0.5232
C	5.2295	2.4428	-0.1126	C	-2.3689	-2.9368	-0.4929	H	1.9824	3.1555	-0.9238
C	5.1178	1.1234	0.2059	C	-1.2872	-0.7573	-0.0206	H	4.5904	-1.4879	0.6749
C	2.8657	2.5906	-0.6048	C	-2.4592	-1.5125	-0.3287	H	0.5969	1.1854	-0.6492
C	2.7101	1.2087	-0.2678	C	-3.7053	-0.8964	-0.4086	H	3.2757	-3.4922	0.7585
C	3.8492	0.4678	0.1295	C	-1.4566	0.5834	0.3201	H	1.1264	-4.6642	0.3339
C	3.7053	-0.8964	0.4086	C	-2.7100	1.2087	0.2678	H	-1.1264	-4.6642	-0.3339
C	1.4566	0.5835	-0.3201	C	-3.8492	0.4678	-0.1295	H	-3.2757	-3.4922	-0.7585
C	1.2872	-0.7573	0.0206	C	-5.1178	1.1234	-0.2059	H	-4.5904	-1.4880	-0.6749
C	2.4592	-1.5125	0.3287	C	-5.2295	2.4428	0.1126	H	-0.5970	1.1855	0.6493
C	2.3688	-2.9368	0.4929	C	-4.0885	3.1852	0.5273	H	-5.9900	0.5410	-0.5233
C	1.1955	-3.5715	0.2763	C	-2.8657	2.5906	0.6048	H	-6.1970	2.9524	0.0564
C	-0.0000	-1.4361	0.0000	H	4.2134	4.2426	-0.7822	H	-4.2135	4.2426	0.7822
C	-0.0000	-2.8271	0.0000	H	6.1970	2.9523	-0.0565	H	-1.9824	3.1555	0.9238

Table 3.282: Table of thermodynamic data as a function of temperature for Anthra[1,2-*a*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.674	458.198	458.198	∞
100	108.910	346.924	775.399	-42.848	484.860	533.225	-278.522
200	214.245	452.896	587.685	-26.958	470.722	587.228	-153.365
250	275.681	507.253	566.136	-14.721	464.095	617.123	-128.938
298.15	335.635	560.948	560.948	0.000	458.198	647.145	-113.375
300	337.911	563.031	560.954	0.623	457.981	648.316	-112.880
350	397.760	619.660	565.290	19.030	452.549	680.480	-101.554
400	453.261	676.452	575.637	40.326	447.838	713.363	-93.154
450	503.542	732.794	589.976	64.268	443.764	746.803	-86.685
500	548.498	788.220	607.038	90.591	440.243	780.687	-81.556
600	623.950	895.164	646.227	149.363	434.554	849.340	-73.940
700	683.735	996.010	689.068	214.859	430.449	918.822	-68.562
800	731.802	1090.560	733.409	285.720	427.740	988.780	-64.559
900	771.076	1179.096	778.065	360.928	426.245	1058.998	-61.461
1000	803.598	1262.072	822.361	439.711	425.799	1129.336	-58.989
1100	830.815	1339.977	865.913	521.471	426.203	1199.686	-56.967
1200	853.781	1413.280	908.503	605.733	427.314	1269.949	-55.278
1300	873.294	1482.410	950.016	692.112	428.952	1340.108	-53.845
1400	889.974	1547.755	990.400	780.297	430.985	1410.130	-52.612
1500	904.313	1609.658	1029.638	870.029	433.329	1479.996	-51.537
1600	916.702	1668.426	1067.742	961.095	435.856	1549.690	-50.591
1700	927.460	1724.331	1104.734	1053.315	438.493	1619.199	-49.751
1800	936.845	1777.615	1140.647	1146.541	441.165	1688.614	-49.001
1900	945.071	1828.492	1175.521	1240.646	443.839	1757.829	-48.325
2000	952.311	1877.156	1209.395	1335.522	446.462	1826.930	-47.714
2100	958.710	1923.778	1242.311	1431.080	448.957	1895.888	-47.157
2200	964.388	1968.510	1274.310	1527.240	451.324	1964.734	-46.648
2300	969.446	2011.493	1305.433	1623.937	453.554	2033.473	-46.181
2400	973.968	2052.849	1335.720	1721.112	455.581	2102.074	-45.750
2500	978.024	2092.692	1365.207	1818.715	457.414	2170.703	-45.353
2600	981.674	2131.124	1393.930	1916.703	459.019	2239.151	-44.984
2700	984.970	2168.235	1421.925	2015.038	460.397	2307.610	-44.642
2800	987.954	2204.111	1449.223	2113.687	461.526	2376.046	-44.325
2900	990.664	2238.828	1475.855	2212.620	462.375	2444.393	-44.027
3000	993.131	2272.455	1501.851	2311.811	462.987	2512.740	-43.750
3100	995.383	2305.057	1527.238	2411.239	463.286	2580.999	-43.489
3200	997.444	2336.692	1552.041	2510.881	463.313	2649.323	-43.245
3300	999.334	2367.414	1576.286	2610.722	463.049	2717.688	-43.017
3400	1001.072	2397.274	1599.996	2710.743	462.469	2785.983	-42.801
3500	1002.673	2426.316	1623.192	2810.932	461.575	2854.282	-42.597
3600	1004.151	2454.583	1645.896	2911.274	460.389	2922.693	-42.406
3700	1005.517	2482.114	1668.126	3011.758	458.882	2991.161	-42.227
3800	1006.784	2508.947	1689.901	3112.374	457.026	3059.612	-42.056
3900	1007.959	2535.114	1711.239	3213.112	454.861	3128.070	-41.895
4000	1009.052	2560.647	1732.156	3313.963	452.373	3196.720	-41.744
4100	1010.070	2585.576	1752.669	3414.920	449.525	3265.365	-41.600
4200	1011.020	2609.928	1772.791	3515.975	446.346	3334.075	-41.464
4300	1011.907	2633.728	1792.537	3617.122	442.821	3402.778	-41.335
4400	1012.737	2657.001	1811.920	3718.354	438.960	3471.656	-41.213
4500	1013.514	2679.769	1830.954	3819.667	434.775	3540.681	-41.098
4600	1014.243	2702.053	1849.649	3921.055	430.217	3609.808	-40.990
4700	1014.929	2723.873	1868.018	4022.514	425.300	3678.929	-40.886
4800	1015.573	2745.247	1886.072	4124.040	420.069	3748.259	-40.789
4900	1016.179	2766.194	1903.821	4225.628	414.453	3817.573	-40.695
5000	1016.751	2786.729	1921.274	4327.275	408.542	3887.186	-40.608

3.283. Naphtho[2,1-*c*]chrysene



Other names: Benzo[*c*]pentahelicene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 58029-44-0

Point Group: C₁

Length: 14.04 Å

Width: 10.68 Å

Breadth: 5.887 Å

L/B Ratio: 1.315

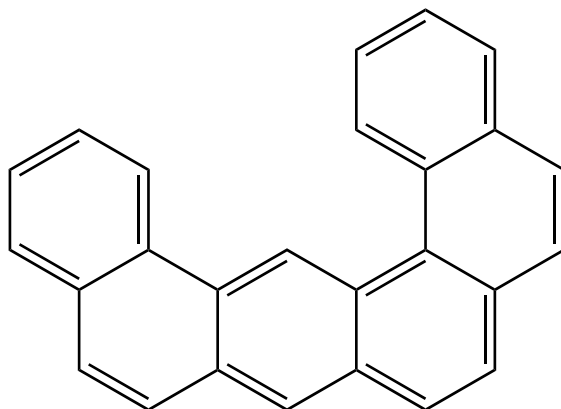
Cartesian coordinates:

C	-2.7564	-3.6304	0.7456	C	0.6690	3.0904	0.6831	H	-0.1693	-1.2549	-1.2926
C	-3.6605	-2.8559	0.0611	C	1.8295	2.3806	0.7055	H	-0.8724	-3.6671	1.8129
C	-1.2703	-1.7410	0.9577	C	0.6723	0.4167	-0.1735	H	-5.3341	-1.1168	-1.1020
C	-1.5644	-3.0567	1.2232	C	1.8629	1.0435	0.2151	H	-5.0184	1.3525	-1.1617
C	-2.1528	-0.9340	0.1989	C	1.9435	-1.4498	-1.0871	H	-3.7564	3.3006	-0.5446
C	-3.3897	-1.4898	-0.1857	C	0.7554	-0.8249	-0.8858	H	-1.6556	4.3420	0.2998
C	-4.4022	-0.6548	-0.7570	C	3.1583	-0.8901	-0.5801	H	0.6502	4.1472	0.9732
C	-4.2222	0.6885	-0.8058	C	3.1240	0.3601	0.0619	H	2.7717	2.8330	1.0504
C	-1.8827	0.4593	-0.0824	C	4.3351	0.9170	0.5367	H	1.9948	-2.3917	-1.6453
C	-2.9768	1.2719	-0.4083	C	5.5226	0.2440	0.3839	H	-0.3453	-1.2977	1.3495
C	-2.8760	2.6906	-0.3125	C	5.5511	-1.0100	-0.2550	H	4.3013	1.9003	1.0299
C	-1.7204	3.2627	0.1212	C	4.3901	-1.5683	-0.7317	H	6.4560	0.6777	0.7572
C	-0.5874	1.0849	0.0320	H	-2.9634	-4.6877	0.9401	H	6.5061	-1.5331	-0.3685
C	-0.5502	2.4660	0.2904	H	-4.6088	-3.2813	-0.2867	H	4.4028	-2.5427	-1.2332

Table 3.283: Table of thermodynamic data as a function of temperature for Naphtho[2,1-c]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-49.482	460.832	460.832	∞
100	108.559	348.032	775.609	-42.758	487.584	535.838	-279.887
200	213.778	453.716	588.267	-26.910	473.404	589.746	-154.023
250	275.189	507.965	566.755	-14.697	466.753	619.603	-129.456
298.15	335.160	561.574	561.574	0.000	460.832	649.593	-113.804
300	337.437	563.654	561.580	0.622	460.614	650.763	-113.306
350	397.350	620.215	565.910	19.007	455.161	682.898	-101.915
400	452.933	676.957	576.247	40.284	450.431	715.754	-93.466
450	503.292	733.266	590.571	64.212	446.343	749.169	-86.960
500	548.313	788.669	607.620	90.524	442.811	783.030	-81.801
600	623.843	895.587	646.784	149.282	437.108	851.640	-74.140
700	683.653	996.418	689.605	214.770	432.994	921.081	-68.730
800	731.718	1090.957	733.930	285.622	430.276	990.998	-64.704
900	770.978	1179.483	778.571	360.821	428.773	1061.177	-61.588
1000	803.486	1262.448	822.855	439.593	428.315	1131.477	-59.101
1100	830.691	1340.342	866.395	521.341	428.708	1201.790	-57.067
1200	853.649	1413.634	908.975	605.590	429.806	1272.017	-55.368
1300	873.158	1482.753	950.479	691.956	431.431	1342.142	-53.927
1400	889.838	1548.087	990.853	780.128	433.450	1412.129	-52.686
1500	904.177	1609.981	1030.084	869.846	435.780	1481.963	-51.605
1600	916.569	1668.740	1068.179	960.898	438.294	1551.625	-50.654
1700	927.331	1724.637	1105.164	1053.106	440.918	1621.103	-49.809
1800	936.722	1777.914	1141.070	1146.319	443.577	1690.487	-49.056
1900	944.952	1828.785	1175.937	1240.411	446.240	1759.673	-48.376
2000	952.198	1877.443	1209.805	1335.276	448.851	1828.744	-47.761
2100	958.603	1924.059	1242.715	1430.823	451.335	1897.674	-47.201
2200	964.286	1968.787	1274.708	1526.973	453.691	1966.492	-46.690
2300	969.349	2011.765	1305.826	1623.660	455.912	2035.204	-46.220
2400	973.876	2053.118	1336.107	1720.825	457.929	2103.778	-45.787
2500	977.937	2092.957	1365.589	1818.419	459.753	2172.381	-45.388
2600	981.592	2131.385	1394.308	1916.399	461.349	2240.802	-45.017
2700	984.892	2168.493	1422.299	2014.726	462.720	2309.235	-44.674
2800	987.880	2204.366	1449.593	2113.367	463.841	2377.645	-44.355
2900	990.593	2239.081	1476.221	2212.293	464.683	2445.967	-44.056
3000	993.064	2272.705	1502.213	2311.477	465.287	2514.289	-43.777
3100	995.319	2305.305	1527.596	2410.898	465.580	2582.523	-43.514
3200	997.383	2336.938	1552.396	2510.535	465.601	2650.822	-43.269
3300	999.277	2367.659	1576.638	2610.369	465.331	2719.162	-43.040
3400	1001.017	2397.517	1600.344	2710.385	464.745	2787.433	-42.823
3500	1002.621	2426.557	1623.538	2810.568	463.846	2855.708	-42.618
3600	1004.101	2454.823	1646.238	2910.905	462.655	2924.095	-42.427
3700	1005.470	2482.353	1668.465	3011.384	461.143	2992.539	-42.246
3800	1006.738	2509.184	1690.238	3111.996	459.282	3060.967	-42.075
3900	1007.915	2535.350	1711.573	3212.729	457.113	3129.401	-41.913
4000	1009.010	2560.882	1732.488	3313.576	454.620	3198.027	-41.761
4100	1010.030	2585.810	1752.998	3414.529	451.769	3266.648	-41.617
4200	1010.981	2610.161	1773.118	3515.580	448.586	3335.335	-41.480
4300	1011.870	2633.960	1792.862	3616.723	445.057	3404.015	-41.350
4400	1012.701	2657.232	1812.243	3717.952	441.192	3472.870	-41.227
4500	1013.480	2679.999	1831.275	3819.261	437.003	3541.871	-41.112
4600	1014.211	2702.283	1849.968	3920.646	432.442	3610.975	-41.003
4700	1014.897	2724.102	1868.335	4022.102	427.522	3680.073	-40.899
4800	1015.542	2745.476	1886.387	4123.624	422.288	3749.381	-40.801
4900	1016.150	2766.422	1904.134	4225.209	416.669	3818.672	-40.707
5000	1016.723	2786.957	1921.586	4326.853	410.755	3888.262	-40.620

3.284. Benzo[*a*]naphth[2,1-*j*]anthracene



Other names: Dibenzo[*a,m*]tetraphene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 58029-41-7

Point Group: C₁

Length: 14.35 Å

Width: 10.91 Å

Breadth: 5.042 Å

L/B Ratio: 1.315

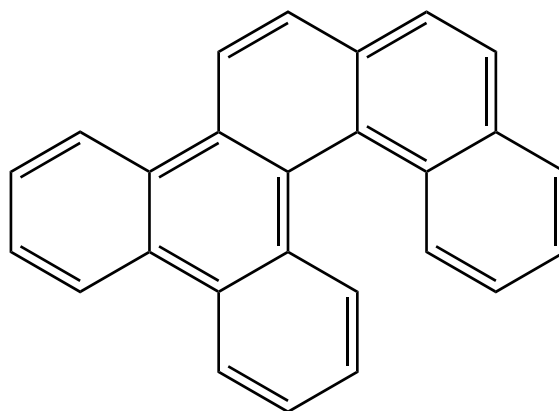
Cartesian coordinates:

C	-1.7489	-1.8270	0.6822	C	1.0832	2.7273	0.2771	H	1.5510	-2.2327	-0.4382
C	-2.5087	-0.7588	0.1412	C	2.1093	1.7900	0.2095	H	3.4212	-3.8690	-0.6474
C	-3.8530	-1.0335	-0.1936	C	1.7863	0.4279	-0.0038	H	5.5354	1.5819	0.3026
C	-4.3597	-2.3537	-0.1103	C	0.4490	0.0465	-0.0877	H	3.7059	3.2490	0.5010
C	-3.5738	-3.3733	0.3618	C	3.4897	2.1890	0.3243	H	1.3260	3.7902	0.4027
C	-2.2619	-3.0958	0.7877	C	4.4846	1.2821	0.2158	H	0.2384	-1.0205	-0.2808
C	-4.7337	0.0257	-0.5684	C	4.1952	-0.1102	-0.0185	H	-0.9886	4.3912	0.2336
C	-4.3005	1.3112	-0.5284	C	2.8615	-0.5403	-0.1287	H	-3.3421	3.7510	-0.2433
C	-2.9379	1.6087	-0.2220	C	5.2413	-1.0456	-0.1375	H	-4.9823	2.1407	-0.7496
C	-2.0057	0.5894	-0.0079	C	4.9624	-2.3775	-0.3613	H	-5.7648	-0.2168	-0.8500
C	-2.5607	2.9900	-0.1331	C	3.6334	-2.8096	-0.4703	H	-5.3943	-2.5446	-0.4182
C	-1.2780	3.3411	0.1120	C	2.5990	-1.9054	-0.3550	H	-3.9603	-4.3953	0.4279
C	-0.2565	2.3354	0.1679	H	5.7766	-3.1035	-0.4552	H	-1.6541	-3.9021	1.2117
C	-0.6018	0.9631	0.0479	H	6.2791	-0.7037	-0.0517	H	-0.7290	-1.6389	1.0451

Table 3.284: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphth[2,1-*j*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.680	438.780	438.780	∞
100	109.343	352.824	781.026	-42.820	465.470	513.245	-268.086
200	214.066	458.888	593.492	-26.921	451.342	566.650	-147.991
250	275.285	513.180	571.974	-14.698	444.700	596.246	-124.576
298.15	335.112	566.794	566.794	0.000	438.780	625.985	-109.668
300	337.385	568.874	566.800	0.622	438.562	627.145	-109.193
350	397.186	625.418	571.129	19.001	433.103	659.019	-98.351
400	452.693	682.133	581.461	40.268	428.363	691.616	-90.314
450	503.005	738.410	595.780	64.183	424.262	724.774	-84.128
500	548.001	793.781	612.821	90.480	420.714	758.378	-79.226
600	623.528	900.641	651.965	149.206	414.980	826.480	-71.950
700	683.368	1001.426	694.764	214.663	410.836	895.418	-66.816
800	731.473	1095.930	739.068	285.489	408.092	964.836	-62.996
900	770.773	1184.429	783.689	360.665	406.566	1034.518	-60.041
1000	803.317	1267.374	827.955	439.419	406.090	1104.325	-57.683
1100	830.551	1345.253	871.479	521.152	406.467	1174.146	-55.754
1200	853.534	1418.534	914.044	605.388	407.553	1243.883	-54.144
1300	873.063	1487.645	955.534	691.744	409.166	1313.518	-52.777
1400	889.759	1552.973	995.897	779.907	411.177	1383.017	-51.600
1500	904.111	1614.861	1035.116	869.618	413.500	1452.362	-50.575
1600	916.514	1673.617	1073.202	960.664	416.008	1521.536	-49.672
1700	927.284	1729.511	1110.178	1052.866	418.627	1590.527	-48.870
1800	936.682	1782.785	1146.077	1146.075	421.281	1659.424	-48.154
1900	944.918	1833.654	1180.936	1240.164	423.940	1728.122	-47.508
2000	952.168	1882.310	1214.798	1335.026	426.548	1796.707	-46.924
2100	958.577	1928.925	1247.702	1430.570	429.030	1865.150	-46.392
2200	964.264	1973.652	1279.690	1526.717	431.383	1933.482	-45.906
2300	969.329	2016.629	1310.802	1623.402	433.602	2001.707	-45.459
2400	973.858	2057.981	1341.079	1720.565	435.617	2069.795	-45.047
2500	977.921	2097.820	1370.556	1818.158	437.440	2137.911	-44.668
2600	981.578	2136.247	1399.271	1916.136	439.034	2205.846	-44.315
2700	984.879	2173.355	1427.258	2014.461	440.404	2273.793	-43.988
2800	987.868	2209.227	1454.548	2113.101	441.523	2341.717	-43.684
2900	990.583	2243.941	1481.174	2212.026	442.364	2409.553	-43.400
3000	993.054	2277.566	1507.163	2311.210	442.968	2477.389	-43.134
3100	995.311	2310.165	1532.543	2410.630	443.260	2545.137	-42.884
3200	997.376	2341.798	1557.340	2510.265	443.280	2612.950	-42.651
3300	999.269	2372.518	1581.579	2610.099	443.009	2680.804	-42.433
3400	1001.010	2402.376	1605.283	2710.114	442.422	2748.589	-42.226
3500	1002.614	2431.416	1628.474	2810.296	441.523	2816.378	-42.031
3600	1004.095	2459.682	1651.172	2910.633	440.331	2884.279	-41.849
3700	1005.464	2487.212	1673.398	3011.112	438.818	2952.237	-41.677
3800	1006.733	2514.043	1695.168	3111.722	436.957	3020.179	-41.514
3900	1007.911	2540.208	1716.502	3212.455	434.788	3088.127	-41.360
4000	1009.006	2565.741	1737.415	3313.302	432.294	3156.268	-41.216
4100	1010.026	2590.668	1757.923	3414.254	429.442	3224.403	-41.079
4200	1010.977	2615.019	1778.042	3515.305	426.259	3292.604	-40.949
4300	1011.866	2638.818	1797.784	3616.447	422.730	3360.798	-40.825
4400	1012.698	2662.090	1817.164	3717.676	418.864	3429.168	-40.709
4500	1013.477	2684.857	1836.194	3818.985	414.676	3497.683	-40.599
4600	1014.208	2707.140	1854.886	3920.370	410.114	3566.301	-40.496
4700	1014.894	2728.960	1873.252	4021.825	405.194	3634.913	-40.397
4800	1015.540	2750.333	1891.303	4123.347	399.960	3703.735	-40.304
4900	1016.148	2771.279	1909.048	4224.932	394.340	3772.540	-40.215
5000	1016.721	2791.814	1926.499	4326.576	388.426	3841.645	-40.133

3.285. Dibenzo[*c,g*]chrysene



Other names: Benzo[*f*]pentahelicene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 53156-66-4

Point Group: C₁

Length: 13.74 Å

Width: 10.24 Å

Breadth: 6.324 Å

L/B Ratio: 1.341

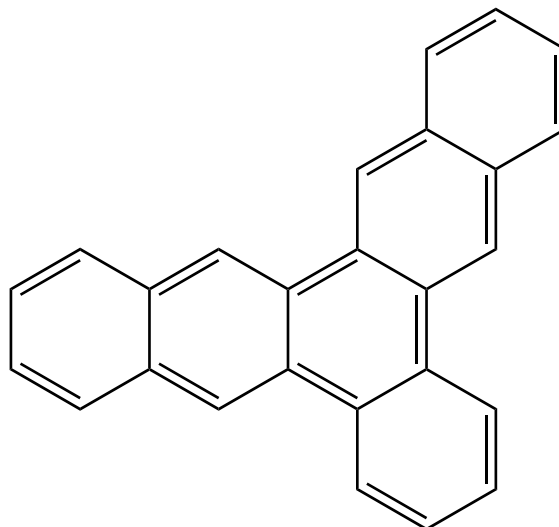
Cartesian coordinates:

C	-4.1587	0.7351	-0.5597	C	1.2410	-0.8246	0.1669	H	1.1323	1.4684	-1.3251
C	-2.8507	0.3692	-0.1922	C	2.3465	-0.0033	-0.2870	H	-3.2945	2.9908	0.1669
C	-2.5013	-0.9895	-0.1454	C	2.1537	1.1648	-1.0613	H	0.7283	-4.1511	0.8433
C	-3.4830	-1.9581	-0.4289	C	1.5289	-2.1587	0.5021	H	-1.6115	-3.4831	0.2855
C	-4.7633	-1.5835	-0.7814	C	0.4845	-3.1114	0.5972	H	4.9462	-2.0124	0.7413
C	-5.1016	-0.2273	-0.8565	C	-0.8022	-2.7384	0.3274	H	3.0554	-3.5914	1.1056
C	-1.1291	-1.3721	0.1396	C	3.6683	-0.4356	-0.0615	H	1.3321	1.6030	1.3512
C	-0.1274	-0.3979	0.2238	C	3.9123	-1.7221	0.5228	H	3.0569	2.8124	-2.0969
C	-0.5432	0.9785	0.4592	C	2.8817	-2.5740	0.7365	H	5.3775	2.1434	-1.5101
C	-1.8719	1.3642	0.2052	C	3.2235	1.9117	-1.4969	H	5.7769	0.0309	-0.2578
C	0.3200	1.9153	1.0624	C	4.5366	1.5249	-1.1805	H	-3.2092	-3.0224	-0.3681
C	-0.0893	3.2114	1.3015	C	4.7563	0.3619	-0.4815	H	-5.5173	-2.3451	-1.0054
C	-1.3809	3.6172	0.9482	H	-1.6921	4.6537	1.1121	H	-6.1162	0.0653	-1.1454
C	-2.2629	2.6995	0.4179	H	0.5962	3.9256	1.7694	H	-4.4155	1.8050	-0.5934

Table 3.285: Table of thermodynamic data as a function of temperature for Dibenzo[*c,g*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.645	464.932	464.932	∞
100	109.817	348.139	776.744	-42.860	491.582	539.824	-281.970
200	214.239	454.516	589.105	-26.918	477.496	593.679	-155.050
250	275.229	508.819	567.593	-14.693	470.857	623.493	-130.269
298.15	334.974	562.414	562.414	0.000	464.932	653.442	-114.478
300	337.246	564.493	562.420	0.622	464.714	654.610	-113.975
350	397.063	621.016	566.748	18.994	459.248	686.704	-102.483
400	452.627	677.718	577.077	40.257	454.503	719.522	-93.958
450	503.001	733.991	591.392	64.170	450.400	752.900	-87.393
500	548.046	789.365	608.429	90.468	446.854	786.725	-82.187
600	623.621	896.238	647.571	149.201	441.127	855.268	-74.456
700	683.457	997.038	690.370	214.668	436.992	924.645	-68.996
800	731.532	1091.552	734.675	285.501	434.255	994.502	-64.933
900	770.795	1180.056	779.298	360.681	432.733	1064.622	-61.788
1000	803.306	1263.002	823.566	439.436	432.258	1134.866	-59.278
1100	830.513	1340.878	867.091	521.166	432.632	1205.124	-57.225
1200	853.475	1414.154	909.657	605.397	433.713	1275.299	-55.511
1300	872.989	1483.260	951.148	691.746	435.320	1345.372	-54.057
1400	889.676	1548.582	991.510	779.901	437.323	1415.310	-52.805
1500	904.023	1610.465	1030.729	869.604	439.638	1485.094	-51.715
1600	916.422	1669.215	1068.814	960.641	442.137	1554.709	-50.755
1700	927.192	1725.103	1105.789	1052.834	444.746	1624.140	-49.903
1800	936.590	1778.372	1141.687	1146.033	447.391	1693.478	-49.142
1900	944.828	1829.236	1176.545	1240.113	450.041	1762.618	-48.457
2000	952.081	1877.888	1210.405	1334.966	452.640	1831.645	-47.837
2100	958.492	1924.498	1243.307	1430.501	455.113	1900.530	-47.272
2200	964.183	1969.221	1275.294	1526.641	457.459	1969.305	-46.756
2300	969.252	2012.195	1306.405	1623.317	459.669	2037.973	-46.283
2400	973.784	2053.543	1336.680	1720.473	461.677	2106.504	-45.846
2500	977.850	2093.379	1366.156	1818.059	463.493	2175.065	-45.445
2600	981.510	2131.804	1394.869	1916.030	465.080	2243.444	-45.070
2700	984.814	2168.909	1422.854	2014.349	466.443	2311.835	-44.724
2800	987.806	2204.780	1450.143	2112.982	467.556	2380.204	-44.402
2900	990.524	2239.491	1476.767	2211.901	468.391	2448.484	-44.101
3000	992.998	2273.114	1502.754	2311.079	468.989	2516.766	-43.820
3100	995.257	2305.711	1528.133	2410.493	469.275	2584.959	-43.555
3200	997.324	2337.343	1552.929	2510.124	469.290	2653.217	-43.308
3300	999.221	2368.061	1577.167	2609.953	469.015	2721.517	-43.077
3400	1000.964	2397.917	1600.869	2709.963	468.423	2789.748	-42.858
3500	1002.570	2426.956	1624.059	2810.141	467.519	2857.983	-42.652
3600	1004.052	2455.221	1646.756	2910.473	466.323	2926.330	-42.459
3700	1005.423	2482.750	1668.980	3010.947	464.805	2994.734	-42.277
3800	1006.694	2509.580	1690.749	3111.554	462.940	3063.122	-42.105
3900	1007.873	2535.744	1712.082	3212.283	460.767	3131.517	-41.941
4000	1008.970	2561.275	1732.994	3313.126	458.270	3200.104	-41.788
4100	1009.992	2586.202	1753.501	3414.075	455.415	3268.686	-41.643
4200	1010.944	2610.552	1773.618	3515.122	452.228	3337.333	-41.505
4300	1011.835	2634.351	1793.360	3616.261	448.695	3405.974	-41.374
4400	1012.667	2657.622	1812.739	3717.487	444.827	3474.790	-41.250
4500	1013.448	2680.388	1831.768	3818.793	440.635	3543.753	-41.134
4600	1014.179	2702.671	1850.459	3920.175	436.071	3612.818	-41.024
4700	1014.867	2724.489	1868.824	4021.628	431.148	3681.877	-40.919
4800	1015.514	2745.863	1886.874	4123.147	425.911	3751.146	-40.820
4900	1016.122	2766.808	1904.619	4224.729	420.289	3820.398	-40.725
5000	1016.696	2787.342	1922.068	4326.370	414.372	3889.950	-40.637

3.286. Benzo[*h*]pentaphene



Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 214-91-5
Point Group: C_{2v}

Length: 15.89 Å
Width: 11.65 Å
Breadth: 3.885 Å
L/B Ratio: 1.364

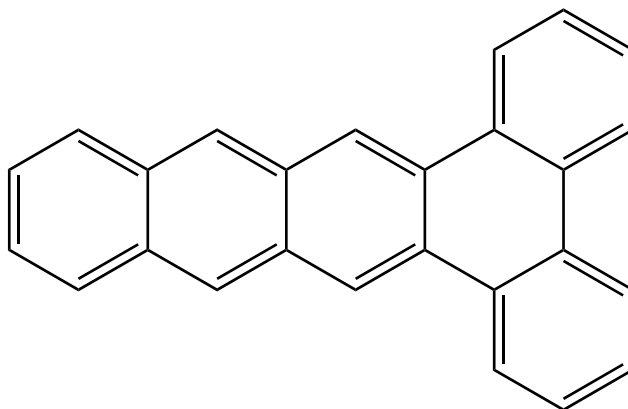
Cartesian coordinates:

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C	4.9734	-0.4002	0.0000	C	-4.9743	-0.3882	0.0000	H	3.3775	1.7805	0.0000
C	3.5739	-2.8302	0.0000	C	-5.6516	-1.5751	0.0000	H	0.8869	-2.5443	0.0000
C	2.8456	-1.6066	0.0000	C	-4.9473	-2.8050	0.0000	H	-3.3732	1.7886	0.0000
C	3.5496	-0.3843	0.0000	C	-3.5808	-2.8215	0.0000	H	-0.8930	-2.5421	0.0000
C	2.8242	0.8275	0.0000	C	-0.6998	2.1008	0.0000	H	-5.5111	0.5671	0.0000
C	1.4335	-1.5874	0.0000	C	0.7049	2.0991	0.0000	H	-6.7464	-1.5918	0.0000
C	0.7304	-0.3979	0.0000	C	1.3897	3.3240	0.0000	H	-5.5157	-3.7408	0.0000
C	1.4427	0.8382	0.0000	C	0.7026	4.5254	0.0000	H	-3.0284	-3.7679	0.0000
C	-0.7314	-0.3961	0.0000	C	-0.6916	4.5270	0.0000	H	2.4904	3.3188	0.0000
C	-1.4407	0.8417	0.0000	C	-1.3816	3.3273	0.0000	H	1.2519	5.4723	0.0000
C	-2.8222	0.8343	0.0000	H	5.5066	-3.7542	0.0000	H	-1.2387	5.4753	0.0000
C	-1.4373	-1.5839	0.0000	H	6.7425	-1.6081	0.0000	H	-2.4824	3.3248	0.0000

Table 3.286: Table of thermodynamic data as a function of temperature for Benzo[h]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-50.082	428.939	428.939	∞
100	111.807	351.651	782.073	-43.042	455.407	503.298	-262.891
200	215.029	459.031	593.841	-26.962	441.459	556.738	-145.402
250	275.656	513.469	572.300	-14.708	434.849	586.323	-122.503
298.15	335.159	567.117	567.117	0.000	428.939	616.047	-107.927
300	337.423	569.197	567.123	0.622	428.721	617.206	-107.463
350	397.048	625.732	571.452	18.998	423.259	649.065	-96.866
400	452.464	682.422	581.782	40.256	418.509	681.646	-89.012
450	502.733	738.669	596.096	64.158	414.395	714.790	-82.969
500	547.713	794.011	613.129	90.441	410.834	748.382	-78.181
600	623.243	900.819	652.256	149.138	405.071	816.464	-71.078
700	683.102	1001.561	695.036	214.568	400.899	885.386	-66.067
800	731.229	1096.031	739.320	285.368	398.129	954.793	-62.340
900	770.550	1184.502	783.923	360.521	396.580	1024.466	-59.457
1000	803.114	1267.425	828.172	439.254	396.083	1094.267	-57.157
1100	830.366	1345.286	871.679	520.967	396.440	1164.084	-55.277
1200	853.365	1418.551	914.230	605.186	397.508	1233.818	-53.706
1300	872.909	1487.649	955.707	691.525	399.106	1303.452	-52.372
1400	889.618	1552.966	996.057	779.673	401.102	1372.951	-51.224
1500	903.982	1614.845	1035.265	869.371	403.412	1442.297	-50.224
1600	916.395	1673.593	1073.340	960.404	405.907	1511.474	-49.344
1700	927.175	1729.480	1110.306	1052.595	408.514	1580.467	-48.561
1800	936.581	1782.748	1146.196	1145.794	411.158	1649.367	-47.862
1900	944.825	1833.612	1181.048	1239.873	413.808	1718.070	-47.232
2000	952.082	1882.264	1214.901	1334.726	416.407	1786.659	-46.662
2100	958.497	1928.874	1247.798	1430.261	418.880	1855.107	-46.142
2200	964.190	1973.598	1279.779	1526.401	421.226	1923.444	-45.667
2300	969.261	2016.572	1310.885	1623.079	423.437	1991.675	-45.231
2400	973.794	2057.921	1341.156	1720.235	425.446	2059.768	-44.829
2500	977.861	2097.757	1370.628	1817.822	427.263	2127.891	-44.459
2600	981.522	2136.182	1399.338	1915.794	428.851	2195.832	-44.114
2700	984.826	2173.288	1427.319	2014.114	430.215	2263.786	-43.795
2800	987.819	2209.158	1454.605	2112.749	431.330	2331.716	-43.498
2900	990.536	2243.870	1481.226	2211.669	432.166	2399.559	-43.220
3000	993.011	2277.494	1507.211	2310.848	432.765	2467.402	-42.960
3100	995.270	2310.092	1532.587	2410.264	433.053	2535.158	-42.716
3200	997.337	2341.723	1557.381	2509.896	433.068	2602.978	-42.488
3300	999.233	2372.442	1581.616	2609.726	432.794	2670.840	-42.275
3400	1000.976	2402.299	1605.317	2709.737	432.204	2738.632	-42.073
3500	1002.581	2431.338	1628.505	2809.916	431.301	2806.429	-41.883
3600	1004.063	2459.603	1651.200	2910.249	430.106	2874.338	-41.705
3700	1005.434	2487.132	1673.422	3010.725	428.590	2942.304	-41.537
3800	1006.705	2513.962	1695.190	3111.333	426.725	3010.254	-41.378
3900	1007.884	2540.127	1716.521	3212.063	424.554	3078.211	-41.227
4000	1008.980	2565.659	1737.432	3312.907	422.057	3146.359	-41.086
4100	1010.001	2590.586	1757.938	3413.856	419.203	3214.503	-40.952
4200	1010.954	2614.936	1778.054	3514.905	416.017	3282.712	-40.826
4300	1011.844	2638.735	1797.794	3616.045	412.486	3350.914	-40.705
4400	1012.676	2662.006	1817.172	3717.272	408.618	3419.292	-40.591
4500	1013.456	2684.772	1836.199	3818.579	404.427	3487.816	-40.485
4600	1014.188	2707.055	1854.890	3919.961	399.864	3556.443	-40.384
4700	1014.875	2728.874	1873.254	4021.415	394.941	3625.063	-40.287
4800	1015.521	2750.247	1891.303	4122.935	389.706	3693.894	-40.197
4900	1016.130	2771.193	1909.047	4224.518	384.084	3762.707	-40.110
5000	1016.704	2791.727	1926.496	4326.160	378.168	3831.821	-40.030

3.287. Dibenzo[*a,c*]naphthacene



Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 216-00-2
Point Group: C_{2v}

Length: 16.03 Å
Width: 11.38 Å
Breadth: 3.886 Å
L/B Ratio: 1.409

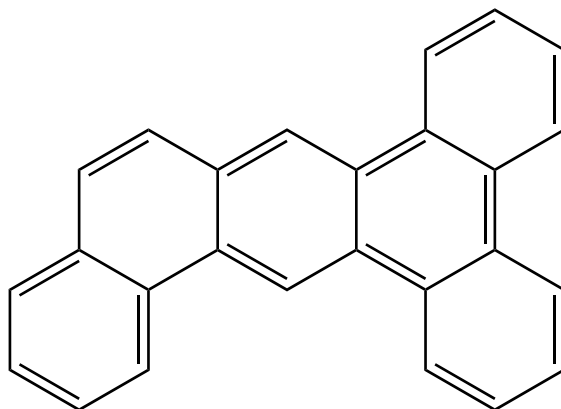
Cartesian coordinates:

C	-6.4728	0.7107	0.0000	C	2.0925	1.4367	0.0000	H	-5.2918	-2.5028	0.0000
C	-6.4722	-0.7162	0.0000	C	3.3073	0.7311	0.0000	H	-5.2939	2.4982	0.0000
C	-5.3022	-1.4069	0.0000	C	4.5144	1.4471	0.0000	H	-2.8349	-2.5032	0.0000
C	-5.3034	1.4024	0.0000	C	4.5216	2.8306	0.0000	H	-2.8370	2.5007	0.0000
C	-4.0463	0.7104	0.0000	C	3.3157	3.5315	0.0000	H	-0.3766	-2.4986	0.0000
C	-4.0457	-0.7139	0.0000	C	2.1173	2.8402	0.0000	H	-0.3788	2.4982	0.0000
C	-2.8368	-1.4063	0.0000	C	3.3080	-0.7282	0.0000	H	5.4637	0.8899	0.0000
C	-2.8380	1.4038	0.0000	C	2.0938	-1.4349	0.0000	H	5.4714	3.3751	0.0000
C	-1.6207	0.7093	0.0000	C	2.1199	-2.8384	0.0000	H	3.3185	4.6262	0.0000
C	-1.6201	-0.7108	0.0000	C	3.3190	-3.5286	0.0000	H	1.1629	3.3887	0.0000
C	-0.3729	-1.3965	0.0000	C	4.5243	-2.8266	0.0000	H	1.1660	-3.3879	0.0000
C	-0.3741	1.3961	0.0000	C	4.5158	-1.4431	0.0000	H	3.3229	-4.6234	0.0000
C	0.8209	0.7185	0.0000	H	-7.4345	1.2342	0.0000	H	5.4746	-3.3702	0.0000
C	0.8216	-0.7179	0.0000	H	-7.4334	-1.2405	0.0000	H	5.4646	-0.8850	0.0000

Table 3.287: Table of thermodynamic data as a function of temperature for Dibenz[*a,c*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-50.055	441.628	441.628	∞
100	111.522	351.837	781.955	-43.012	468.127	516.000	-269.525
200	214.938	459.032	593.816	-26.957	454.154	569.433	-148.718
250	275.619	513.458	572.279	-14.705	447.541	599.018	-125.155
298.15	335.079	567.097	567.097	0.000	441.628	628.742	-110.151
300	337.340	569.176	567.103	0.622	441.410	629.902	-109.673
350	396.888	625.693	571.431	18.992	435.942	661.762	-98.761
400	452.232	682.357	581.757	40.240	431.183	694.346	-90.670
450	502.449	738.574	596.064	64.129	427.056	727.494	-84.444
500	547.395	793.883	613.090	90.397	423.479	761.092	-79.509
600	622.901	900.630	652.196	149.060	417.683	829.189	-72.186
700	682.767	1001.320	694.954	214.456	413.477	898.133	-67.018
800	730.914	1095.746	739.216	285.224	410.675	967.566	-63.174
900	770.260	1184.182	783.797	360.347	409.095	1037.270	-60.200
1000	802.848	1267.076	828.024	439.052	408.570	1107.104	-57.828
1100	830.124	1344.912	871.513	520.740	408.902	1176.957	-55.888
1200	853.145	1418.157	914.045	604.935	409.947	1246.730	-54.268
1300	872.708	1487.238	955.505	691.253	411.524	1316.404	-52.893
1400	889.434	1552.541	995.840	779.382	413.501	1385.945	-51.709
1500	903.815	1614.408	1035.033	869.062	415.793	1455.334	-50.678
1600	916.242	1673.146	1073.096	960.080	418.272	1524.555	-49.771
1700	927.035	1729.024	1110.049	1052.256	420.865	1593.593	-48.964
1800	936.452	1782.284	1145.928	1145.441	423.496	1662.540	-48.245
1900	944.706	1833.141	1180.769	1239.508	426.132	1731.289	-47.595
2000	951.973	1881.787	1214.612	1334.350	428.720	1799.926	-47.008
2100	958.395	1928.393	1247.500	1429.874	431.183	1868.421	-46.473
2200	964.096	1973.111	1279.473	1526.005	433.519	1936.807	-45.985
2300	969.173	2016.081	1310.571	1622.673	435.721	2005.086	-45.536
2400	973.713	2057.427	1340.834	1719.821	437.722	2073.229	-45.122
2500	977.785	2097.260	1370.300	1817.400	439.530	2141.401	-44.741
2600	981.451	2135.682	1399.003	1915.365	441.111	2209.393	-44.386
2700	984.760	2172.785	1426.978	2013.678	442.469	2277.396	-44.058
2800	987.756	2208.654	1454.258	2112.306	443.577	2345.377	-43.753
2900	990.478	2243.363	1480.874	2211.220	444.407	2413.271	-43.467
3000	992.956	2276.985	1506.853	2310.394	445.000	2481.165	-43.200
3100	995.218	2309.581	1532.225	2409.804	445.283	2548.971	-42.949
3200	997.287	2341.211	1557.014	2509.431	445.293	2616.843	-42.715
3300	999.186	2371.929	1581.245	2609.256	445.014	2684.756	-42.495
3400	1000.932	2401.783	1604.941	2709.263	444.419	2752.600	-42.288
3500	1002.539	2430.822	1628.125	2809.438	443.512	2820.448	-42.092
3600	1004.024	2459.085	1650.816	2909.767	442.313	2888.409	-41.909
3700	1005.397	2486.613	1673.035	3010.239	440.793	2956.426	-41.736
3800	1006.669	2513.442	1694.800	3110.843	438.925	3024.428	-41.573
3900	1007.850	2539.607	1716.127	3211.569	436.750	3092.437	-41.418
4000	1008.948	2565.137	1737.035	3312.410	434.250	3160.638	-41.273
4100	1009.970	2590.063	1757.538	3413.356	431.393	3228.833	-41.135
4200	1010.924	2614.413	1777.651	3514.402	428.204	3297.095	-41.005
4300	1011.815	2638.211	1797.388	3615.539	424.670	3365.350	-40.880
4400	1012.649	2661.482	1816.763	3716.763	420.799	3433.780	-40.763
4500	1013.430	2684.248	1835.788	3818.067	416.606	3502.356	-40.653
4600	1014.163	2706.530	1854.476	3919.447	412.040	3571.035	-40.550
4700	1014.851	2728.348	1872.838	4020.898	407.115	3639.708	-40.450
4800	1015.498	2749.721	1890.884	4122.416	401.876	3708.591	-40.357
4900	1016.108	2770.666	1908.626	4223.997	396.253	3777.458	-40.267
5000	1016.682	2791.200	1926.073	4325.636	390.335	3846.624	-40.185

3.288. Naphtho[1,2-*b*]triphenylene



Other names: Dibenzo[*f,m*]tetraphene
 Tribenz[*a,c,h*]anthracene
 1,2,3,4,5,6-Tribenzanthracene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 215-26-9
Point Group: C_s

Length: 15.68 Å
Width: 11.14 Å
Breadth: 3.886 Å
L/B Ratio: 1.407

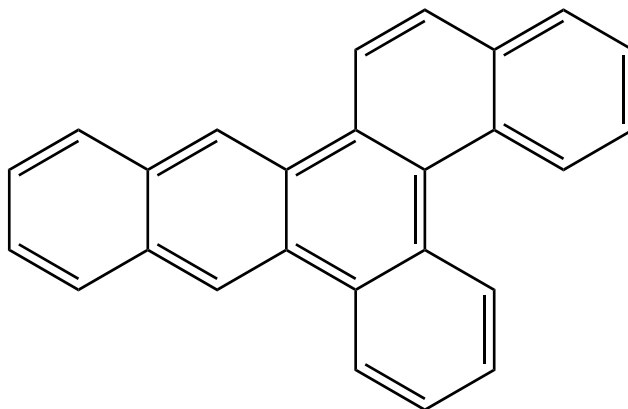
Cartesian coordinates:

C	5.9639	-0.9066	0.0000	C	-1.5569	-1.4549	0.0000	H	2.8650	-2.3472	0.0000
C	5.5972	0.4215	0.0000	C	-2.9085	-1.0718	0.0000	H	5.2859	-2.9621	0.0000
C	3.6475	-1.5728	0.0000	C	-3.9020	-2.0660	0.0000	H	4.6352	2.9273	0.0000
C	4.9828	-1.9101	0.0000	C	-3.5653	-3.4060	0.0000	H	2.2389	3.5767	0.0000
C	3.2502	-0.2202	0.0000	C	-2.2212	-3.7870	0.0000	H	-0.1213	2.9574	0.0000
C	4.2344	0.7834	0.0000	C	-1.2320	-2.8224	0.0000	H	1.1141	-1.8757	0.0000
C	3.8442	2.1685	0.0000	C	-3.2666	0.3400	0.0000	H	-4.9591	-1.7590	0.0000
C	2.5388	2.5224	0.0000	C	-2.2613	1.3216	0.0000	H	-4.3493	-4.1702	0.0000
C	1.8515	0.1562	0.0000	C	-2.6287	2.6783	0.0000	H	-1.9546	-4.8488	0.0000
C	1.5033	1.5229	0.0000	C	-3.9583	3.0539	0.0000	H	-0.1706	-3.1147	0.0000
C	0.1518	1.8897	0.0000	C	-4.9578	2.0779	0.0000	H	-1.8359	3.4420	0.0000
C	0.8334	-0.8048	0.0000	C	-4.6141	0.7397	0.0000	H	-4.2306	4.1143	0.0000
C	-0.5099	-0.4420	0.0000	H	7.0223	-1.1870	0.0000	H	-6.0114	2.3754	0.0000
C	-0.8576	0.9311	0.0000	H	6.3601	1.2083	0.0000	H	-5.3966	-0.0345	0.0000

Table 3.288: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*b*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.961	415.744	415.744	∞
100	111.678	358.902	787.606	-42.870	442.383	489.550	-255.709
200	214.131	465.883	600.143	-26.852	428.374	542.283	-141.627
250	274.524	520.095	578.689	-14.648	421.713	571.530	-119.412
298.15	333.839	573.526	573.526	0.000	415.744	600.940	-105.280
300	336.098	575.599	573.533	0.620	415.523	602.088	-104.831
350	395.607	631.920	577.845	18.926	409.992	633.632	-94.562
400	450.980	688.414	588.137	40.111	405.168	665.909	-86.957
450	501.259	744.486	602.400	63.939	400.980	698.758	-81.108
500	546.279	799.675	619.377	90.149	397.346	732.063	-76.477
600	621.931	906.231	658.384	148.708	391.446	799.591	-69.609
700	681.919	1006.781	701.048	214.013	387.149	867.982	-64.768
800	730.161	1101.100	745.223	284.701	384.267	936.875	-61.170
900	769.583	1189.452	789.727	359.753	382.616	1006.048	-58.388
1000	802.235	1272.278	833.885	438.393	382.027	1075.359	-56.170
1100	829.566	1350.058	877.311	520.023	382.300	1144.694	-54.356
1200	852.634	1423.257	919.787	604.164	383.292	1213.955	-52.841
1300	872.240	1492.299	961.196	690.434	384.820	1283.121	-51.555
1400	889.005	1557.568	1001.484	778.518	386.751	1352.157	-50.449
1500	903.420	1619.407	1040.636	868.157	389.002	1421.046	-49.484
1600	915.878	1678.120	1078.660	959.137	391.444	1489.768	-48.635
1700	926.699	1733.977	1115.578	1051.278	394.002	1558.310	-47.880
1800	936.142	1787.219	1151.424	1144.431	396.600	1626.762	-47.206
1900	944.419	1838.060	1186.235	1238.468	399.207	1695.018	-46.598
2000	951.706	1886.692	1220.051	1333.282	401.767	1763.164	-46.048
2100	958.148	1933.285	1252.913	1428.781	404.204	1831.170	-45.547
2200	963.865	1977.992	1284.862	1524.887	406.517	1899.066	-45.089
2300	968.959	2020.952	1315.938	1621.533	408.697	1966.859	-44.668
2400	973.512	2062.289	1346.180	1718.661	410.676	2034.514	-44.279
2500	977.598	2102.114	1375.626	1816.220	412.466	2102.201	-43.922
2600	981.275	2140.529	1404.311	1914.167	414.028	2169.707	-43.589
2700	984.595	2177.626	1432.269	2012.463	415.369	2237.227	-43.281
2800	987.602	2213.488	1459.533	2111.075	416.461	2304.724	-42.994
2900	990.332	2248.193	1486.133	2209.974	417.276	2372.134	-42.726
3000	992.818	2281.809	1512.098	2309.134	417.855	2439.545	-42.475
3100	995.088	2314.401	1537.456	2408.531	418.124	2506.869	-42.240
3200	997.165	2346.027	1562.232	2508.145	418.122	2574.259	-42.020
3300	999.070	2376.741	1586.451	2607.958	417.831	2641.691	-41.814
3400	1000.821	2406.593	1610.136	2707.953	417.225	2709.054	-41.619
3500	1002.435	2435.628	1633.308	2808.117	416.307	2776.421	-41.435
3600	1003.924	2463.888	1655.989	2908.436	415.098	2843.901	-41.263
3700	1005.302	2491.414	1678.198	3008.898	413.568	2911.439	-41.101
3800	1006.579	2518.241	1699.953	3109.493	411.691	2978.961	-40.948
3900	1007.764	2544.403	1721.271	3210.211	409.507	3046.490	-40.802
4000	1008.866	2569.931	1742.170	3311.043	406.999	3114.211	-40.667
4100	1009.892	2594.855	1762.665	3411.982	404.133	3181.927	-40.537
4200	1010.849	2619.203	1782.770	3513.019	400.937	3249.709	-40.415
4300	1011.744	2642.999	1802.499	3614.150	397.395	3317.485	-40.299
4400	1012.580	2666.268	1821.867	3715.366	393.518	3385.437	-40.189
4500	1013.364	2689.033	1840.885	3816.664	389.317	3453.535	-40.087
4600	1014.100	2711.314	1859.566	3918.037	384.745	3521.735	-39.990
4700	1014.790	2733.131	1877.922	4019.482	379.814	3589.930	-39.897
4800	1015.440	2754.502	1895.962	4120.994	374.570	3658.335	-39.810
4900	1016.052	2775.446	1913.697	4222.569	368.941	3726.723	-39.727
5000	1016.628	2795.979	1931.138	4324.203	363.017	3795.412	-39.650

3.289. Dibenzo[*b,p*]chrysene



Other names: Dibenzo[*c,f*]tetraphene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 58029-42-8

Point Group: C₁

Length: 15.97 Å

Width: 11.14 Å

Breadth: 5.055 Å

L/B Ratio: 1.434

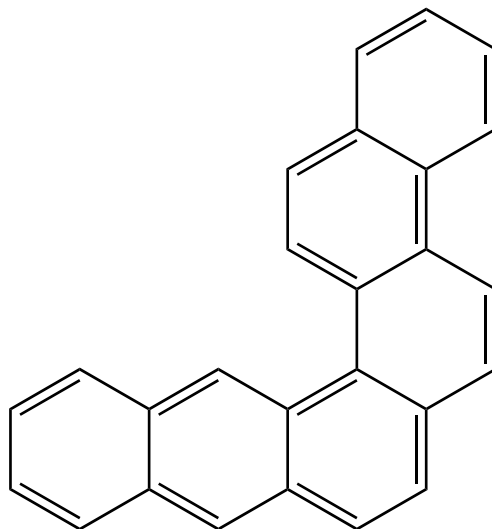
Cartesian coordinates:

C	5.6274	-1.7297	-0.1137	C	-3.1290	-1.8513	0.1546	H	5.2123	1.6259	-0.6272
C	5.9512	-0.3731	-0.3766	C	-2.8383	-0.4930	-0.1003	H	4.0728	-3.1511	0.2944
C	4.9717	0.5761	-0.4255	C	-3.8904	0.3035	-0.6270	H	2.8300	2.2297	-0.4205
C	4.3316	-2.1057	0.0919	C	-5.1536	-0.1980	-0.8038	H	1.6952	-2.5564	0.4280
C	3.2858	-1.1370	0.0449	C	-5.4478	-1.5337	-0.4632	H	-2.3303	-3.7855	0.7586
C	3.6089	0.2137	-0.2127	C	-4.4490	-2.3478	-0.0003	H	0.0256	-3.0084	0.7440
C	2.5777	1.1720	-0.2426	C	-1.1462	1.4121	0.1557	H	-3.6862	1.3451	-0.9101
C	1.9386	-1.4987	0.2398	C	0.1992	1.8076	0.0238	H	-5.9456	0.4353	-1.2171
C	0.9244	-0.5558	0.1862	C	0.5301	3.1737	0.0214	H	-6.4682	-1.9106	-0.5859
C	1.2572	0.8101	-0.0347	C	-0.4355	4.1410	0.2172	H	-4.6517	-3.3964	0.2463
C	-0.4780	-0.9412	0.2847	C	-1.7559	3.7523	0.4467	H	1.5814	3.4643	-0.1277
C	-1.4960	-0.0067	0.1075	C	-2.0984	2.4136	0.4186	H	-0.1666	5.2020	0.2110
C	-2.0842	-2.7438	0.5231	H	6.4348	-2.4685	-0.0793	H	-2.5201	4.5093	0.6514
C	-0.7962	-2.3078	0.5320	H	6.9996	-0.1020	-0.5390	H	-3.1437	2.1349	0.6103

Table 3.289: Table of thermodynamic data as a function of temperature for Dibenzo[*b,p*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.860	450.928	450.928	∞
100	110.715	352.748	782.482	-42.973	477.465	525.247	-274.355
200	214.749	459.633	594.433	-26.960	463.450	578.609	-151.114
250	275.651	514.040	572.890	-14.712	456.834	608.165	-127.066
298.15	335.347	567.704	567.704	0.000	450.928	637.861	-111.748
300	337.617	569.786	567.711	0.622	450.711	639.020	-111.261
350	397.386	626.362	572.043	19.012	445.262	670.848	-100.116
400	452.899	683.104	582.381	40.290	440.532	703.397	-91.852
450	503.227	739.407	596.706	64.215	436.441	736.505	-85.489
500	548.234	794.802	613.755	90.523	432.906	770.059	-80.446
600	623.755	901.705	652.918	149.272	427.195	838.056	-72.958
700	683.561	1002.522	695.735	214.751	423.071	906.886	-67.671
800	731.622	1097.049	740.056	285.594	420.345	976.193	-63.738
900	770.878	1185.563	784.693	360.783	418.831	1045.763	-60.693
1000	803.384	1268.518	828.972	439.545	418.364	1115.456	-58.264
1100	830.588	1346.402	872.508	521.283	418.746	1185.162	-56.278
1200	853.547	1419.684	915.083	605.522	419.834	1254.784	-54.618
1300	873.059	1488.796	956.582	691.878	421.448	1324.304	-53.210
1400	889.742	1554.123	996.952	780.039	423.458	1393.688	-51.998
1500	904.086	1616.010	1036.177	869.749	425.779	1462.918	-50.942
1600	916.482	1674.763	1074.269	960.792	428.284	1531.978	-50.013
1700	927.249	1730.655	1111.249	1052.991	430.899	1600.854	-49.187
1800	936.644	1783.927	1147.152	1146.196	433.550	1669.636	-48.451
1900	944.879	1834.795	1182.015	1240.281	436.205	1738.221	-47.786
2000	952.128	1883.449	1215.879	1335.139	438.809	1806.692	-47.185
2100	958.537	1930.061	1248.786	1430.678	441.287	1875.021	-46.638
2200	964.224	1974.786	1280.776	1526.822	443.636	1943.239	-46.137
2300	969.291	2017.762	1311.891	1623.503	445.851	2011.351	-45.678
2400	973.821	2059.112	1342.169	1720.662	447.863	2079.325	-45.254
2500	977.885	2098.949	1371.649	1818.251	449.682	2147.329	-44.865
2600	981.543	2137.375	1400.365	1916.226	451.272	2215.151	-44.502
2700	984.845	2174.482	1428.353	2014.548	452.638	2282.986	-44.166
2800	987.836	2210.353	1455.644	2113.185	453.755	2350.797	-43.854
2900	990.552	2245.066	1482.270	2212.106	454.592	2418.520	-43.561
3000	993.025	2278.689	1508.260	2311.287	455.193	2486.243	-43.288
3100	995.282	2311.288	1533.641	2410.704	455.482	2553.879	-43.032
3200	997.348	2342.920	1558.439	2510.337	455.499	2621.580	-42.792
3300	999.243	2373.639	1582.679	2610.168	455.226	2689.322	-42.568
3400	1000.985	2403.496	1606.384	2710.180	454.637	2756.995	-42.355
3500	1002.590	2432.535	1629.575	2810.360	453.735	2824.672	-42.155
3600	1004.072	2460.800	1652.274	2910.694	452.541	2892.461	-41.968
3700	1005.442	2488.330	1674.500	3011.171	451.025	2960.307	-41.791
3800	1006.712	2515.160	1696.271	3111.779	449.162	3028.137	-41.624
3900	1007.890	2541.325	1717.605	3212.510	446.991	3095.974	-41.465
4000	1008.986	2566.857	1738.518	3313.355	444.495	3164.003	-41.317
4100	1010.007	2591.784	1759.027	3414.305	441.641	3232.027	-41.176
4200	1010.959	2616.134	1779.145	3515.354	438.456	3300.116	-41.042
4300	1011.849	2639.933	1798.888	3616.495	434.925	3368.199	-40.915
4400	1012.681	2663.205	1818.268	3717.722	431.058	3436.456	-40.795
4500	1013.461	2685.972	1837.298	3819.029	426.868	3504.860	-40.683
4600	1014.192	2708.254	1855.991	3920.412	422.305	3573.367	-40.576
4700	1014.879	2730.073	1874.357	4021.866	417.383	3641.868	-40.474
4800	1015.525	2751.447	1892.408	4123.387	412.147	3710.578	-40.378
4900	1016.134	2772.393	1910.154	4224.970	406.526	3779.272	-40.287
5000	1016.707	2792.927	1927.605	4326.612	400.611	3848.265	-40.202

3.290. Naphtho[2,3-*c*]chrysene



Other names: Naphtho[2,1-*a*]tetraphene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 58029-37-1

Point Group: C₁

Length: 16.27 Å

Width: 10.51 Å

Breadth: 5.029 Å

L/B Ratio: 1.548

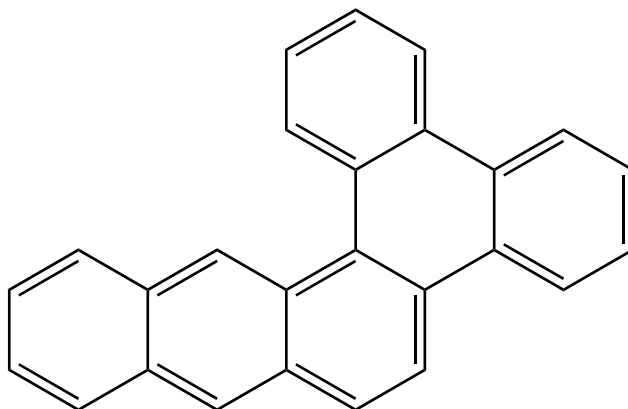
Cartesian coordinates:

C	-4.8147	2.8008	0.4349	C	1.5472	-2.9409	0.2792	H	-6.2675	-0.1968	-0.3449
C	-5.8244	1.8475	0.1313	C	2.6046	-2.0824	0.3564	H	-2.7192	3.1606	0.7119
C	-5.4969	0.5471	-0.1134	C	1.1359	-0.1990	-0.1635	H	-4.5426	-1.9615	-0.4489
C	-3.5032	2.4313	0.4784	C	2.4234	-0.6999	0.1000	H	-1.0228	1.4440	0.4745
C	-3.1252	1.0783	0.2168	C	2.1084	1.9820	-0.6847	H	-2.9068	-3.7119	-0.4729
C	-4.1322	0.1282	-0.0699	C	1.0323	1.1607	-0.6133	H	-0.5721	-4.4675	-0.0849
C	-3.7623	-1.2101	-0.2735	C	3.4078	1.5214	-0.3025	H	1.6940	-4.0197	0.4080
C	-1.7772	0.6811	0.2333	C	3.5710	0.1789	0.0776	H	3.6172	-2.4493	0.5832
C	-1.3930	-0.6268	-0.0390	C	4.8639	-0.2739	0.4297	H	2.0049	3.0128	-1.0432
C	-2.4280	-1.5932	-0.2292	C	5.9377	0.5836	0.4104	H	0.0507	1.5369	-0.9328
C	-2.0975	-2.9934	-0.2989	C	5.7663	1.9280	0.0341	H	4.9921	-1.3277	0.7199
C	-0.8275	-3.4015	-0.1026	C	4.5215	2.3912	-0.3195	H	6.9346	0.2262	0.6882
C	-0.0015	-1.0696	-0.0546	H	-5.1101	3.8364	0.6324	H	6.6315	2.5988	0.0247
C	0.2389	-2.4460	0.0495	H	-6.8681	2.1769	0.0994	H	4.3776	3.4359	-0.6175

Table 3.290: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*c*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.709	447.035	447.035	∞
100	109.331	353.238	781.777	-42.854	473.691	521.424	-272.358
200	214.257	459.371	594.088	-26.943	459.574	574.785	-150.115
250	275.524	513.712	572.553	-14.710	452.943	604.356	-126.271
298.15	335.357	567.368	567.368	0.000	447.035	634.068	-111.084
300	337.630	569.449	567.374	0.623	446.818	635.227	-110.601
350	397.408	626.030	571.706	19.013	441.370	667.072	-99.553
400	452.878	682.772	582.045	40.291	436.640	699.637	-91.361
450	503.153	739.069	596.371	64.214	432.547	732.762	-85.055
500	548.115	794.454	613.419	90.517	429.006	766.333	-80.057
600	623.592	901.330	652.577	149.252	423.281	834.367	-72.637
700	683.400	1002.122	695.388	214.714	419.141	903.236	-67.399
800	731.485	1096.629	739.701	285.542	416.399	972.584	-63.502
900	770.774	1185.129	784.330	360.719	414.874	1042.197	-60.486
1000	803.312	1268.074	828.601	439.473	414.398	1111.934	-58.080
1100	830.543	1345.952	872.130	521.205	414.774	1181.684	-56.112
1200	853.523	1419.232	914.699	605.440	415.859	1251.352	-54.469
1300	873.051	1488.342	956.193	691.794	417.471	1320.917	-53.074
1400	889.747	1553.669	996.558	779.956	419.481	1390.346	-51.873
1500	904.100	1615.557	1035.780	869.666	421.803	1459.621	-50.827
1600	916.502	1674.312	1073.868	960.711	424.310	1528.726	-49.907
1700	927.273	1730.205	1110.845	1052.912	426.927	1597.647	-49.089
1800	936.671	1783.479	1146.745	1146.120	429.581	1666.475	-48.359
1900	944.908	1834.347	1181.606	1240.208	432.239	1735.104	-47.700
2000	952.159	1883.003	1215.469	1335.068	434.845	1803.620	-47.105
2100	958.568	1929.617	1248.374	1430.611	437.326	1871.993	-46.562
2200	964.255	1974.344	1280.363	1526.758	439.679	1940.256	-46.067
2300	969.322	2017.320	1311.476	1623.442	441.897	2008.412	-45.612
2400	973.851	2058.672	1341.753	1720.604	443.911	2076.430	-45.191
2500	977.914	2098.510	1371.232	1818.196	445.733	2144.478	-44.805
2600	981.571	2136.937	1399.947	1916.174	447.327	2212.344	-44.446
2700	984.873	2174.045	1427.934	2014.499	448.696	2280.222	-44.113
2800	987.862	2209.917	1455.225	2113.138	449.815	2348.077	-43.803
2900	990.577	2244.631	1481.851	2212.062	450.655	2415.843	-43.513
3000	993.049	2278.255	1507.840	2311.245	451.258	2483.610	-43.243
3100	995.306	2310.855	1533.221	2410.665	451.550	2551.290	-42.988
3200	997.371	2342.487	1558.019	2510.300	451.569	2619.034	-42.750
3300	999.265	2373.207	1582.258	2610.133	451.298	2686.819	-42.528
3400	1001.006	2403.065	1605.962	2710.148	450.711	2754.535	-42.317
3500	1002.610	2432.105	1629.153	2810.330	449.811	2822.255	-42.119
3600	1004.091	2460.370	1651.852	2910.666	448.619	2890.087	-41.933
3700	1005.461	2487.900	1674.077	3011.144	447.105	2957.976	-41.758
3800	1006.730	2514.731	1695.848	3111.755	445.244	3025.849	-41.592
3900	1007.908	2540.897	1717.182	3212.487	443.074	3093.729	-41.435
4000	1009.003	2566.429	1738.096	3313.333	440.580	3161.801	-41.288
4100	1010.023	2591.356	1758.604	3414.285	437.728	3229.867	-41.148
4200	1010.975	2615.707	1778.722	3515.336	434.545	3297.999	-41.016
4300	1011.864	2639.506	1798.465	3616.478	431.015	3366.125	-40.889
4400	1012.695	2662.778	1817.845	3717.706	427.149	3434.425	-40.771
4500	1013.474	2685.545	1836.875	3819.015	422.960	3502.872	-40.659
4600	1014.205	2707.828	1855.568	3920.400	418.399	3571.421	-40.554
4700	1014.892	2729.648	1873.934	4021.855	413.478	3639.964	-40.453
4800	1015.537	2751.021	1891.984	4123.377	408.244	3708.717	-40.358
4900	1016.145	2771.967	1909.730	4224.961	402.624	3777.454	-40.267
5000	1016.718	2792.502	1927.181	4326.605	396.710	3846.490	-40.183

3.291. Dibenzo[*a,c*]tetraphene



Other names: Dibenzo[*b,g*]chrysene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 53156-67-5

Point Group: C₁

Length: 15.88 Å

Width: 10.40 Å

Breadth: 5.192 Å

L/B Ratio: 1.527

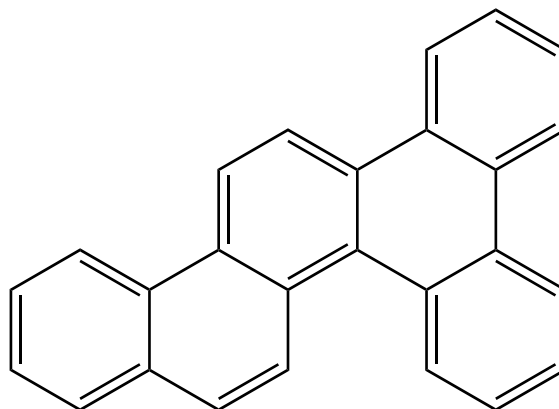
Cartesian coordinates:

C	5.5692	-1.2203	0.6907	C	-1.0324	-1.1785	-0.2469	H	5.6265	2.0454	-0.3311
C	6.0837	0.0535	0.3185	C	-2.4121	-1.3073	0.0091	H	3.8244	-2.4335	0.9672
C	5.2418	1.0598	-0.0457	C	-3.0112	-2.5836	0.0037	H	3.3168	2.8703	-0.6265
C	4.2280	-1.4555	0.6812	C	-2.2844	-3.7078	-0.3171	H	1.5675	-1.6490	0.5454
C	3.3146	-0.4240	0.2942	C	-0.9352	-3.5768	-0.6660	H	1.0742	3.7185	-0.8518
C	3.8273	0.8476	-0.0608	C	-0.3288	-2.3399	-0.6317	H	-1.3662	3.4070	-0.5436
C	2.9312	1.8707	-0.3897	C	-3.2275	-0.1279	0.2137	H	-4.0808	-2.6652	0.2512
C	1.9326	-0.6525	0.2568	C	-2.6548	1.1402	0.0314	H	-2.7564	-4.6954	-0.3177
C	1.0320	0.3395	-0.1298	C	-3.4785	2.2809	0.1402	H	-0.3650	-4.4609	-0.9695
C	1.5579	1.6385	-0.3964	C	-4.8153	2.1632	0.4503	H	0.7289	-2.2627	-0.9189
C	0.6570	2.7350	-0.6073	C	-5.3777	0.8970	0.6621	H	-3.0370	3.2756	-0.0216
C	-0.6742	2.5559	-0.4557	C	-4.5952	-0.2298	0.5413	H	-5.4430	3.0562	0.5361
C	-0.4077	0.1355	-0.1926	H	6.2729	-2.0061	0.9841	H	-6.4385	0.8096	0.9184
C	-1.2293	1.2556	-0.2077	H	7.1676	0.2076	0.3323	H	-5.0298	-1.2298	0.6911

Table 3.291: Table of thermodynamic data as a function of temperature for Dibenzo[*a,c*]tetraphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.785	455.980	455.980	∞
100	110.284	352.540	781.548	-42.901	482.589	530.392	-277.042
200	214.429	459.145	593.779	-26.927	468.535	583.791	-152.467
250	275.319	513.480	572.261	-14.695	461.902	613.373	-128.155
298.15	334.967	567.082	567.082	0.000	455.980	643.098	-112.666
300	337.235	569.161	567.089	0.622	455.761	644.258	-112.173
350	396.958	625.675	571.415	18.991	450.292	676.118	-100.903
400	452.441	682.358	581.742	40.246	445.540	708.703	-92.545
450	502.756	738.605	596.053	64.148	441.426	741.850	-86.110
500	547.764	793.951	613.085	90.433	437.867	775.445	-81.009
600	623.310	900.770	652.210	149.136	432.110	843.532	-73.434
700	683.154	1001.522	694.990	214.572	427.944	912.459	-68.087
800	731.253	1095.996	739.275	285.377	425.178	981.869	-64.108
900	770.545	1184.469	783.880	360.530	423.630	1051.546	-61.029
1000	803.084	1267.390	828.129	439.261	423.131	1121.350	-58.572
1100	830.317	1345.247	871.637	520.971	423.484	1191.171	-56.563
1200	853.302	1418.507	914.188	605.183	424.547	1260.909	-54.885
1300	872.836	1487.600	955.664	691.516	426.138	1330.548	-53.461
1400	889.539	1552.911	996.014	779.656	428.126	1400.052	-52.235
1500	903.901	1614.785	1035.221	869.346	430.428	1469.404	-51.168
1600	916.313	1673.527	1073.295	960.372	432.915	1538.587	-50.229
1700	927.094	1729.410	1110.260	1052.555	435.514	1607.587	-49.394
1800	936.502	1782.673	1146.148	1145.745	438.150	1676.494	-48.650
1900	944.748	1833.533	1180.998	1239.816	440.792	1745.205	-47.978
2000	952.008	1882.181	1214.850	1334.662	443.383	1813.802	-47.371
2100	958.425	1928.788	1247.745	1430.190	445.849	1882.258	-46.818
2200	964.121	1973.508	1279.725	1526.323	448.188	1950.604	-46.312
2300	969.195	2016.479	1310.829	1622.993	450.393	2018.844	-45.848
2400	973.732	2057.825	1341.098	1720.144	452.395	2086.947	-45.420
2500	977.802	2097.658	1370.569	1817.724	454.205	2155.079	-45.027
2600	981.465	2136.081	1399.277	1915.690	455.788	2223.031	-44.660
2700	984.772	2173.185	1427.257	2014.005	457.147	2290.995	-44.321
2800	987.767	2209.054	1454.542	2112.635	458.256	2358.936	-44.006
2900	990.487	2243.764	1481.161	2211.549	459.087	2426.789	-43.710
3000	992.964	2277.386	1507.144	2310.724	459.681	2494.643	-43.435
3100	995.225	2309.982	1532.519	2410.135	459.965	2562.409	-43.175
3200	997.294	2341.612	1557.312	2509.763	459.976	2630.241	-42.933
3300	999.192	2372.330	1581.546	2609.588	459.698	2698.113	-42.707
3400	1000.937	2402.185	1605.245	2709.596	459.103	2765.917	-42.492
3500	1002.544	2431.224	1628.432	2809.771	458.197	2833.725	-42.290
3600	1004.028	2459.487	1651.126	2910.101	456.998	2901.646	-42.101
3700	1005.401	2487.015	1673.347	3010.573	455.478	2969.623	-41.923
3800	1006.672	2513.845	1695.114	3111.177	453.611	3037.585	-41.754
3900	1007.853	2540.009	1716.444	3211.904	451.436	3105.553	-41.593
4000	1008.951	2565.540	1737.353	3312.745	448.937	3173.714	-41.444
4100	1009.973	2590.466	1757.858	3413.692	446.080	3241.869	-41.301
4200	1010.927	2614.816	1777.973	3514.738	442.891	3310.090	-41.166
4300	1011.818	2638.614	1797.712	3615.875	439.357	3378.305	-41.037
4400	1012.651	2661.885	1817.089	3717.099	435.487	3446.695	-40.917
4500	1013.432	2684.651	1836.116	3818.404	431.293	3515.231	-40.803
4600	1014.165	2706.933	1854.806	3919.784	426.727	3583.870	-40.695
4700	1014.853	2728.751	1873.169	4021.235	421.803	3652.503	-40.592
4800	1015.500	2750.124	1891.217	4122.753	416.565	3721.345	-40.496
4900	1016.109	2771.069	1908.960	4224.334	410.941	3790.171	-40.403
5000	1016.684	2791.603	1926.408	4325.974	405.023	3859.297	-40.317

3.292. Benzo[*f*]picene



Other names: Dibenzo[*a,c*]chrysene
1,2,5,6-Dibenzotetraphene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 58029-47-3
Point Group: C₁

Length: 15.82 Å
Width: 10.45 Å
Breadth: 4.985 Å
L/B Ratio: 1.514

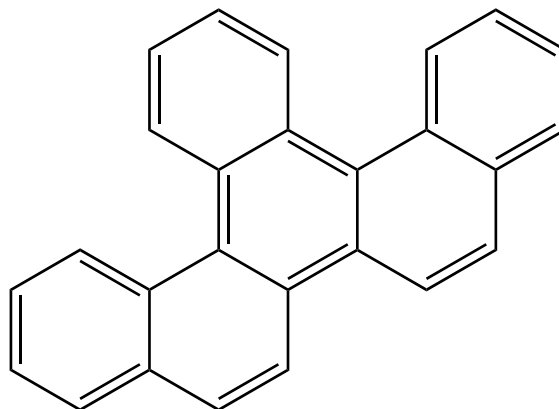
Cartesian coordinates:

C	5.5845	-1.3623	0.2949	C	-2.7336	1.0217	-0.0196	H	5.6252	1.8885	-0.7334
C	6.0951	-0.1139	-0.1032	C	-1.3598	1.2826	0.1521	H	3.8199	-2.5391	0.6802
C	5.2373	0.9130	-0.4189	C	-0.9829	2.5990	0.4846	H	3.3438	2.7187	-1.0522
C	4.2270	-1.5639	0.3729	C	-1.9034	3.6257	0.5405	H	0.9189	2.4253	-0.8314
C	3.3236	-0.5221	0.0602	C	-3.2513	3.3738	0.2703	H	-0.3949	-3.2097	0.5175
C	3.8397	0.7211	-0.3411	C	-3.6580	2.0833	0.0064	H	2.0579	-2.8155	0.6275
C	2.9312	1.7735	-0.6804	C	-2.3032	-1.4017	0.0275	H	0.0689	2.8220	0.7103
C	1.5926	1.6036	-0.5519	C	-3.2075	-0.3438	-0.1491	H	-1.5804	4.6392	0.7999
C	1.8922	-0.7057	0.1420	C	-4.5652	-0.6276	-0.3911	H	-3.9769	4.1932	0.2871
C	1.0186	0.3724	-0.0849	C	-5.0183	-1.9294	-0.4323	H	-4.7211	1.8631	-0.1757
C	0.0138	-2.1972	0.3795	C	-4.1239	-2.9855	-0.2233	H	-5.2635	0.2103	-0.5379
C	1.3619	-1.9887	0.4191	C	-2.7887	-2.7241	0.0027	H	-6.0755	-2.1407	-0.6226
C	-0.8846	-1.1207	0.1721	H	6.2780	-2.1727	0.5424	H	-4.4876	-4.0179	-0.2441
C	-0.3966	0.1882	0.0737	H	7.1788	0.0313	-0.1599	H	-2.0843	-3.5546	0.1608

Table 3.292: Table of thermodynamic data as a function of temperature for Benzo[*f*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.811	444.237	444.237	∞
100	110.629	352.918	781.921	-42.900	470.846	518.611	-270.889
200	214.409	459.641	594.198	-26.911	456.807	571.964	-149.379
250	275.152	513.955	572.694	-14.685	450.170	601.522	-125.679
298.15	334.702	567.519	567.519	0.000	444.237	631.225	-110.586
300	336.968	569.596	567.525	0.621	444.018	632.383	-110.105
350	396.642	626.065	571.849	18.976	438.534	664.224	-99.128
400	452.115	682.705	582.167	40.215	433.765	696.790	-90.990
450	502.439	738.914	596.467	64.101	429.635	729.921	-84.725
500	547.464	794.227	613.487	90.370	426.061	763.501	-79.761
600	623.046	900.994	652.586	149.045	420.276	831.563	-72.393
700	682.915	1001.707	695.342	214.456	416.085	900.470	-67.192
800	731.030	1096.151	739.605	285.237	413.296	969.863	-63.324
900	770.334	1184.599	784.188	360.369	411.726	1039.526	-60.331
1000	802.882	1267.498	828.418	439.080	411.206	1109.318	-57.944
1100	830.124	1345.336	871.909	520.769	411.540	1179.129	-55.991
1200	853.118	1418.580	914.444	604.963	412.584	1248.859	-54.360
1300	872.662	1487.658	955.906	691.278	414.156	1318.491	-52.977
1400	889.375	1552.957	996.242	779.401	416.128	1387.990	-51.785
1500	903.746	1614.820	1035.436	869.075	418.414	1457.338	-50.748
1600	916.168	1673.552	1073.499	960.085	420.886	1526.518	-49.835
1700	926.958	1729.426	1110.453	1052.254	423.471	1595.516	-49.023
1800	936.374	1782.682	1146.331	1145.431	426.094	1664.422	-48.299
1900	944.628	1833.535	1181.171	1239.490	428.723	1733.132	-47.646
2000	951.895	1882.177	1215.015	1334.324	431.303	1801.730	-47.055
2100	958.320	1928.778	1247.901	1429.841	433.758	1870.187	-46.517
2200	964.022	1973.494	1279.874	1525.964	436.086	1938.534	-46.026
2300	969.102	2016.460	1310.971	1622.625	438.282	2006.775	-45.574
2400	973.645	2057.803	1341.233	1719.767	440.275	2074.880	-45.158
2500	977.720	2097.633	1370.697	1817.338	442.077	2143.015	-44.775
2600	981.388	2136.052	1399.400	1915.297	443.651	2210.969	-44.418
2700	984.700	2173.153	1427.374	2013.604	445.003	2278.936	-44.088
2800	987.699	2209.020	1454.653	2112.226	446.105	2346.880	-43.781
2900	990.423	2243.728	1481.267	2211.135	446.929	2414.737	-43.493
3000	992.903	2277.347	1507.246	2310.303	447.517	2482.595	-43.225
3100	995.167	2309.942	1532.616	2409.708	447.795	2550.365	-42.972
3200	997.239	2341.570	1557.404	2509.330	447.800	2618.200	-42.737
3300	999.140	2372.286	1581.635	2609.150	447.517	2686.078	-42.516
3400	1000.887	2402.140	1605.330	2709.153	446.917	2753.886	-42.307
3500	1002.497	2431.177	1628.513	2809.323	446.006	2821.698	-42.111
3600	1003.983	2459.439	1651.203	2909.648	444.803	2889.624	-41.926
3700	1005.358	2486.966	1673.421	3010.116	443.279	2957.606	-41.753
3800	1006.632	2513.794	1695.185	3110.716	441.407	3025.573	-41.589
3900	1007.814	2539.958	1716.512	3211.439	439.228	3093.546	-41.433
4000	1008.913	2565.487	1737.418	3312.276	436.725	3161.712	-41.287
4100	1009.937	2590.413	1757.920	3413.219	433.864	3229.873	-41.148
4200	1010.893	2614.761	1778.032	3514.262	430.672	3298.099	-41.017
4300	1011.785	2638.559	1797.769	3615.396	427.134	3366.319	-40.892
4400	1012.620	2661.829	1817.143	3716.617	423.261	3434.715	-40.774
4500	1013.402	2684.594	1836.168	3817.918	419.065	3503.256	-40.664
4600	1014.136	2706.876	1854.855	3919.295	414.496	3571.901	-40.559
4700	1014.825	2728.693	1873.216	4020.744	409.568	3640.539	-40.459
4800	1015.473	2750.066	1891.262	4122.259	404.328	3709.388	-40.366
4900	1016.084	2771.010	1909.003	4223.837	398.702	3778.220	-40.275
5000	1016.659	2791.544	1926.449	4325.475	392.781	3847.352	-40.192

3.293. Benzo[*s*]picene



Other names: Dibenzo[*a,p*]chrysene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 31540-94-0

Point Group: C₂

Length: 16.01 Å

Width: 10.47 Å

Breadth: 4.748 Å

L/B Ratio: 1.529

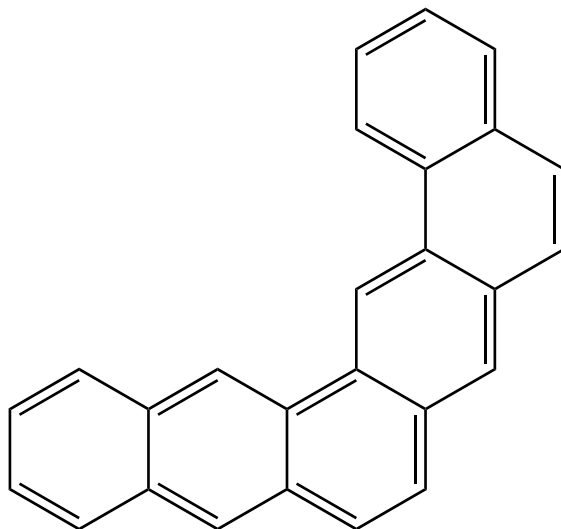
Cartesian coordinates:

C	-5.0906	0.8691	-0.4439	C	-0.6625	3.6715	0.2293	H	-5.3999	-2.3932	0.4656
C	-5.7121	-0.3437	-0.0942	C	-1.3241	2.4752	0.3782	H	-3.2709	1.9418	-0.7103
C	-4.9375	-1.4289	0.2248	C	1.4453	-0.0074	-0.0666	H	-3.2478	-3.4481	0.6447
C	-3.7236	0.9882	-0.4073	C	0.7202	-1.1984	-0.0757	H	-0.7947	-3.3627	0.3585
C	-2.8896	-0.0895	-0.0128	C	1.3936	-2.4428	-0.2837	H	2.3662	2.4914	-0.7219
C	-3.5248	-1.3261	0.2308	C	2.7415	-2.5013	-0.4234	H	1.1658	4.6184	-0.4463
C	-2.7414	-2.5014	0.4240	C	2.8898	-0.0892	0.0124	H	-1.1674	4.6179	0.4478
C	-1.3934	-2.4429	0.2845	C	3.5250	-1.3259	-0.2308	H	-2.3668	2.4898	0.7233
C	-1.4452	-0.0077	0.0666	C	4.9377	-1.4289	-0.2250	H	0.7950	-3.3627	-0.3573
C	-0.7200	-1.1986	0.0761	C	5.7125	-0.3436	0.0933	H	3.2480	-3.4480	-0.6437
C	-0.6995	1.2366	0.1041	C	5.0910	0.8694	0.4425	H	5.3998	-2.3933	-0.4656
C	0.6993	1.2368	-0.1038	C	3.7241	0.9886	0.4061	H	6.8047	-0.4154	0.0983
C	1.3232	2.4759	-0.3774	H	-5.7088	1.7187	-0.7527	H	5.7094	1.7191	0.7507
C	0.6611	3.6718	-0.2282	H	-6.8043	-0.4155	-0.0995	H	3.2719	1.9427	0.7085

Table 3.293: Table of thermodynamic data as a function of temperature for Benzo[s]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-49.586	484.448	484.448	∞
100	109.406	343.756	771.910	-42.815	511.143	559.824	-292.416
200	214.004	449.930	584.436	-26.901	497.029	614.129	-160.391
250	275.059	504.187	562.935	-14.687	490.379	644.174	-134.590
298.15	334.881	557.758	557.758	0.000	484.448	674.347	-118.140
300	337.156	559.837	557.765	0.622	484.230	675.524	-117.617
350	397.049	616.352	562.091	18.991	478.762	707.851	-105.639
400	452.672	673.056	572.419	40.255	474.017	740.901	-96.750
450	503.087	729.337	586.734	64.171	469.918	774.512	-89.901
500	548.157	784.721	603.773	90.474	466.377	808.570	-84.469
600	623.739	891.616	642.918	149.219	460.662	877.576	-76.398
700	683.549	992.432	685.723	214.697	456.537	947.415	-70.696
800	731.586	1086.956	730.034	285.538	453.808	1017.732	-66.450
900	770.813	1175.464	774.662	360.721	452.290	1088.311	-63.163
1000	803.291	1258.410	818.934	439.476	451.814	1159.014	-60.539
1100	830.474	1336.284	862.463	521.203	452.186	1229.732	-58.394
1200	853.417	1409.556	905.031	605.430	453.262	1300.366	-56.602
1300	872.920	1478.657	946.524	691.772	454.863	1370.899	-55.082
1400	889.598	1543.973	986.888	779.920	456.858	1441.297	-53.774
1500	903.940	1605.851	1026.108	869.614	459.165	1511.543	-52.636
1600	916.338	1664.595	1064.193	960.643	461.655	1581.619	-51.633
1700	927.108	1720.478	1101.168	1052.828	464.256	1651.512	-50.744
1800	936.507	1773.742	1137.065	1146.019	466.893	1721.313	-49.950
1900	944.747	1824.602	1171.923	1240.090	469.535	1790.916	-49.235
2000	952.002	1873.250	1205.782	1334.935	472.126	1860.407	-48.588
2100	958.416	1919.856	1238.684	1430.463	474.591	1929.756	-47.999
2200	964.109	1964.576	1270.669	1526.595	476.929	1998.995	-47.461
2300	969.182	2007.546	1301.779	1623.264	479.133	2068.128	-46.968
2400	973.717	2048.892	1332.053	1720.413	481.134	2137.124	-46.512
2500	977.786	2088.725	1361.528	1817.992	482.942	2206.150	-46.094
2600	981.449	2127.147	1390.240	1915.957	484.523	2274.995	-45.704
2700	984.756	2164.250	1418.224	2014.270	485.880	2343.852	-45.344
2800	987.751	2200.118	1445.512	2112.898	486.988	2412.687	-45.008
2900	990.471	2234.828	1472.135	2211.811	487.817	2481.434	-44.695
3000	992.948	2268.449	1498.121	2310.984	488.410	2550.181	-44.402
3100	995.209	2301.045	1523.499	2410.393	488.692	2618.841	-44.126
3200	997.279	2332.675	1548.294	2510.019	488.702	2687.566	-43.869
3300	999.177	2363.392	1572.531	2609.843	488.422	2756.333	-43.628
3400	1000.922	2393.247	1596.232	2709.849	487.826	2825.031	-43.400
3500	1002.530	2422.285	1619.421	2810.023	486.918	2893.732	-43.186
3600	1004.014	2450.548	1642.117	2910.351	485.718	2962.547	-42.985
3700	1005.387	2478.076	1664.340	3010.822	484.197	3031.418	-42.795
3800	1006.659	2504.905	1686.109	3111.425	482.328	3100.274	-42.615
3900	1007.840	2531.069	1707.440	3212.151	480.151	3169.136	-42.445
4000	1008.938	2556.599	1728.351	3312.991	477.651	3238.191	-42.286
4100	1009.961	2581.525	1748.858	3413.936	474.793	3307.240	-42.134
4200	1010.915	2605.874	1768.974	3514.980	471.603	3376.356	-41.990
4300	1011.806	2629.672	1788.715	3616.117	468.067	3445.464	-41.853
4400	1012.640	2652.943	1808.093	3717.340	464.196	3514.748	-41.725
4500	1013.421	2675.708	1827.121	3818.643	460.002	3584.179	-41.603
4600	1014.154	2697.990	1845.812	3920.022	455.435	3653.712	-41.488
4700	1014.843	2719.809	1864.176	4021.473	450.509	3723.239	-41.378
4800	1015.490	2741.181	1882.225	4122.990	445.270	3792.976	-41.275
4900	1016.100	2762.126	1899.969	4224.569	439.646	3862.696	-41.176
5000	1016.674	2782.660	1917.418	4326.208	433.727	3932.716	-41.084

3.294. Benzo[*a*]pentaphene



Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 7689-57-8
Point Group: C_s

Length: 16.14 Å
Width: 10.72 Å
Breadth: 3.889 Å
L/B Ratio: 1.505

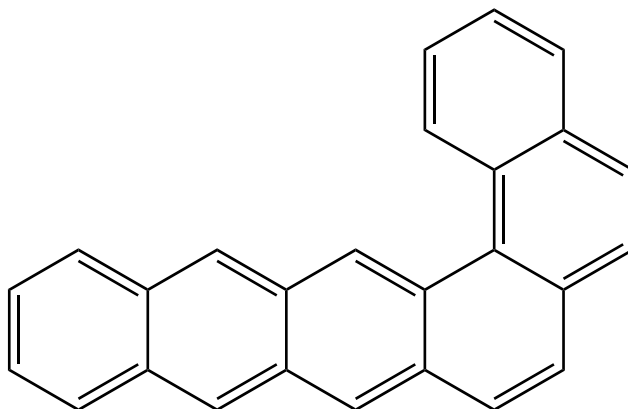
Cartesian coordinates:

C	5.1498	-2.7235	0.0000	C	-1.5836	2.5907	0.0000	H	6.4461	0.4410	0.0000
C	6.1096	-1.6778	0.0000	C	-0.8238	-0.0936	0.0000	H	3.0674	-3.2394	0.0000
C	5.7118	-0.3724	0.0000	C	-2.1846	0.2341	0.0000	H	4.6343	2.1031	0.0000
C	3.8152	-2.4385	0.0000	C	-2.5671	1.5935	0.0000	H	1.2452	-1.5719	0.0000
C	3.3679	-1.0840	0.0000	C	-3.9646	1.9394	0.0000	H	2.8579	3.7613	0.0000
C	4.3240	-0.0420	0.0000	C	-4.9177	0.9802	0.0000	H	0.4465	4.3316	0.0000
C	3.8888	1.2982	0.0000	C	-3.2086	-0.7910	0.0000	H	-1.8843	3.6460	0.0000
C	1.9960	-0.7651	0.0000	C	-4.5628	-0.4145	0.0000	H	-0.5249	-1.1596	0.0000
C	1.5723	0.5531	0.0000	C	-5.5618	-1.4093	0.0000	H	-4.2326	3.0023	0.0000
C	2.5377	1.6011	0.0000	C	-5.2152	-2.7429	0.0000	H	-5.9823	1.2414	0.0000
C	2.0918	2.9771	0.0000	C	-3.8639	-3.1210	0.0000	H	-6.6160	-1.1096	0.0000
C	0.7806	3.2875	0.0000	C	-2.8763	-2.1609	0.0000	H	-5.9916	-3.5149	0.0000
C	0.1562	0.8941	0.0000	H	5.4988	-3.7613	0.0000	H	-3.5999	-4.1836	0.0000
C	-0.2325	2.2560	0.0000	H	7.1734	-1.9370	0.0000	H	-1.8114	-2.4404	0.0000

Table 3.294: Table of thermodynamic data as a function of temperature for Benzo[*a*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.915	418.195	418.195	∞
100	110.275	355.797	785.582	-42.979	444.726	492.203	-257.095
200	214.849	462.475	597.432	-26.991	430.685	545.276	-142.408
250	276.008	516.935	575.862	-14.732	424.081	574.688	-120.072
298.15	335.763	570.670	570.670	0.000	418.195	604.243	-105.859
300	338.032	572.754	570.677	0.623	417.978	605.396	-105.407
350	397.735	629.391	575.013	19.032	412.549	637.074	-95.076
400	453.134	686.172	585.361	40.324	407.833	669.471	-87.422
450	503.349	742.495	599.698	64.259	403.751	702.425	-81.534
500	548.265	797.899	616.757	90.571	400.219	735.824	-76.869
600	623.689	904.797	655.935	149.317	394.506	803.512	-69.950
700	683.483	1005.603	698.762	214.788	390.375	872.033	-65.071
800	731.574	1100.120	743.089	285.625	387.642	941.033	-61.442
900	770.875	1188.631	787.730	360.811	386.126	1010.296	-58.635
1000	803.424	1271.588	832.013	439.575	385.660	1079.682	-56.396
1100	830.664	1349.477	875.551	521.319	386.048	1149.081	-54.564
1200	853.650	1422.768	918.129	605.567	387.145	1218.395	-53.034
1300	873.181	1491.888	959.631	691.934	388.771	1287.606	-51.736
1400	889.876	1557.225	1000.005	780.108	390.793	1356.680	-50.617
1500	904.226	1619.121	1039.234	869.831	393.128	1425.600	-49.643
1600	916.626	1677.884	1077.329	960.889	395.647	1494.348	-48.784
1700	927.392	1733.785	1114.313	1053.102	398.277	1562.911	-48.021
1800	936.785	1787.065	1150.220	1146.321	400.942	1631.380	-47.340
1900	945.017	1837.940	1185.087	1240.420	403.611	1699.651	-46.726
2000	952.262	1886.601	1218.955	1335.292	406.229	1767.807	-46.169
2100	958.666	1933.220	1251.866	1430.845	408.719	1835.820	-45.663
2200	964.348	1977.951	1283.860	1527.001	411.082	1903.722	-45.199
2300	969.410	2020.932	1314.978	1623.694	413.308	1971.517	-44.774
2400	973.935	2062.287	1345.260	1720.865	415.332	2039.174	-44.381
2500	977.993	2102.129	1374.743	1818.465	417.162	2106.860	-44.020
2600	981.646	2140.559	1403.462	1916.450	418.763	2174.365	-43.683
2700	984.944	2177.669	1431.453	2014.783	420.139	2241.880	-43.371
2800	987.930	2213.544	1458.748	2113.429	421.265	2309.372	-43.081
2900	990.641	2248.260	1485.377	2212.359	422.112	2376.776	-42.809
3000	993.110	2281.886	1511.370	2311.549	422.722	2444.180	-42.556
3100	995.364	2314.488	1536.754	2410.974	423.019	2511.496	-42.318
3200	997.426	2346.122	1561.555	2510.615	423.044	2578.877	-42.095
3300	999.317	2376.844	1585.797	2610.454	422.779	2646.299	-41.887
3400	1001.056	2406.703	1609.505	2710.474	422.196	2713.651	-41.689
3500	1002.658	2435.744	1632.699	2810.660	421.301	2781.007	-41.503
3600	1004.136	2464.011	1655.400	2911.001	420.114	2848.475	-41.329
3700	1005.504	2491.542	1677.628	3011.484	418.605	2916.000	-41.166
3800	1006.771	2518.374	1699.401	3112.099	416.747	2983.509	-41.010
3900	1007.947	2544.541	1720.737	3212.835	414.582	3051.024	-40.863
4000	1009.041	2570.074	1741.653	3313.685	412.092	3118.732	-40.726
4100	1010.059	2595.003	1762.163	3414.641	409.244	3186.433	-40.595
4200	1011.009	2619.354	1782.284	3515.695	406.064	3254.201	-40.471
4300	1011.897	2643.154	1802.028	3616.841	402.537	3321.961	-40.353
4400	1012.727	2666.427	1821.410	3718.072	398.675	3389.897	-40.242
4500	1013.505	2689.194	1840.442	3819.384	394.489	3457.979	-40.138
4600	1014.235	2711.478	1859.137	3920.772	389.930	3526.163	-40.040
4700	1014.920	2733.298	1877.504	4022.230	385.013	3594.341	-39.946
4800	1015.565	2754.672	1895.557	4123.754	379.781	3662.729	-39.858
4900	1016.172	2775.619	1913.304	4225.342	374.164	3731.101	-39.773
5000	1016.744	2796.154	1930.757	4326.988	368.252	3799.771	-39.695

3.295. Naphtho[1,2-*a*]naphthacene



Other names: Naphtho[1,2-*a*]tetracene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 58029-39-3

Point Group: C₁

Length: 16.15 Å

Width: 10.32 Å

Breadth: 4.856 Å

L/B Ratio: 1.564

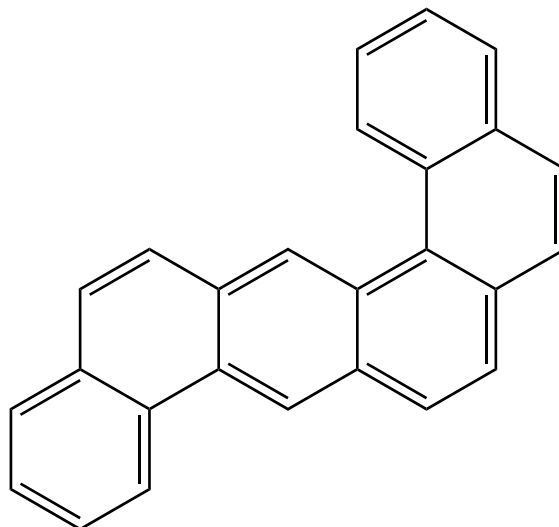
Cartesian coordinates:

C	6.0897	1.5744	-0.3084	C	-1.3102	-3.1335	0.2253	H	5.9928	-1.7682	0.4316
C	6.5429	0.2552	0.0015	C	-2.6157	-2.9092	-0.0203	H	4.4064	2.8509	-0.6522
C	5.6551	-0.7531	0.1939	C	-2.2869	-0.4604	-0.0104	H	3.6634	-2.5505	0.5094
C	4.7635	1.8423	-0.4148	C	-3.1214	-1.5670	-0.1652	H	2.0790	2.0760	-0.5543
C	3.7890	0.8046	-0.2177	C	-4.5095	-1.4115	-0.4468	H	1.3276	-3.3357	0.4842
C	4.2419	-0.5136	0.0898	C	-5.0643	-0.1727	-0.5190	H	-0.2162	1.3176	-0.4335
C	3.3199	-1.5347	0.2782	C	-2.9068	0.8385	0.0991	H	-0.9281	-4.1465	0.3960
C	2.4283	1.0631	-0.3187	C	-4.2795	0.9750	-0.2066	H	-3.3298	-3.7388	-0.0827
C	1.4883	0.0355	-0.1181	C	-4.9037	2.2475	-0.1590	H	-5.1159	-2.3082	-0.6206
C	1.9411	-1.2785	0.1725	C	-4.2037	3.3518	0.2495	H	-6.1204	-0.0396	-0.7800
C	0.9799	-2.3085	0.3158	C	-2.8591	3.2135	0.6459	H	-5.9589	2.3302	-0.4441
C	0.0952	0.2909	-0.1914	C	-2.2338	1.9954	0.5732	H	-4.6808	4.3363	0.2881
C	-0.8446	-0.6960	0.0265	H	6.8359	2.3616	-0.4574	H	-2.3190	4.0892	1.0209
C	-0.3691	-2.0401	0.2172	H	7.6205	0.0778	0.0795	H	-1.1912	1.9133	0.9093

Table 3.295: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.547	466.829	466.829	∞
100	108.618	350.821	778.707	-42.789	493.551	541.525	-282.858
200	213.961	456.598	591.233	-26.927	479.384	595.150	-155.434
250	275.366	510.889	569.708	-14.705	472.742	624.861	-130.555
298.15	335.282	564.525	564.525	0.000	466.829	654.710	-114.700
300	337.557	566.606	564.532	0.622	466.612	655.874	-114.196
350	397.378	623.179	568.863	19.011	461.162	687.861	-102.656
400	452.866	679.919	579.200	40.287	456.431	720.569	-94.095
450	503.148	736.214	593.525	64.210	452.337	753.837	-87.501
500	548.115	791.599	610.573	90.513	448.797	787.551	-82.273
600	623.605	898.477	649.730	149.248	443.072	855.870	-74.509
700	683.433	999.272	692.540	214.713	438.934	925.024	-69.025
800	731.540	1093.785	736.853	285.545	436.197	994.657	-64.943
900	770.848	1182.292	781.483	360.729	434.678	1064.553	-61.784
1000	803.399	1265.246	825.756	439.490	434.210	1134.574	-59.263
1100	830.640	1343.133	869.286	521.232	434.595	1204.607	-57.201
1200	853.626	1416.421	911.857	605.477	435.690	1274.556	-55.479
1300	873.157	1485.540	953.354	691.842	437.313	1344.401	-54.018
1400	889.852	1550.875	993.722	780.014	439.333	1414.110	-52.760
1500	904.203	1612.770	1032.947	869.734	441.666	1483.665	-51.665
1600	916.603	1671.531	1071.038	960.789	444.183	1553.048	-50.701
1700	927.370	1727.430	1108.018	1053.001	446.810	1622.247	-49.845
1800	936.764	1780.709	1143.922	1146.218	449.473	1691.352	-49.081
1900	944.996	1831.583	1178.786	1240.315	452.140	1760.258	-48.392
2000	952.243	1880.243	1212.651	1335.184	454.755	1829.049	-47.769
2100	958.647	1926.861	1245.559	1430.735	457.244	1897.699	-47.202
2200	964.331	1971.591	1277.551	1526.890	459.605	1966.237	-46.683
2300	969.393	2014.571	1308.667	1623.581	461.830	2034.668	-46.208
2400	973.919	2055.926	1338.946	1720.750	463.852	2102.961	-45.769
2500	977.978	2095.767	1368.427	1818.349	465.680	2171.283	-45.366
2600	981.632	2134.196	1397.145	1916.332	467.280	2239.424	-44.990
2700	984.930	2171.306	1425.135	2014.663	468.655	2307.575	-44.642
2800	987.917	2207.181	1452.428	2113.308	469.779	2375.704	-44.318
2900	990.629	2241.896	1479.055	2212.238	470.625	2443.744	-44.016
3000	993.098	2275.522	1505.047	2311.426	471.233	2511.785	-43.733
3100	995.352	2308.123	1530.429	2410.850	471.529	2579.737	-43.467
3200	997.415	2339.757	1555.229	2510.490	471.553	2647.754	-43.219
3300	999.307	2370.479	1579.470	2610.327	471.287	2715.812	-42.987
3400	1001.046	2400.337	1603.176	2710.346	470.704	2783.801	-42.767
3500	1002.649	2429.378	1626.369	2810.532	469.807	2851.794	-42.560
3600	1004.127	2457.645	1649.069	2910.872	468.619	2919.899	-42.366
3700	1005.495	2485.176	1671.296	3011.354	467.109	2988.060	-42.183
3800	1006.763	2512.008	1693.069	3111.968	465.251	3056.206	-42.010
3900	1007.939	2538.174	1714.404	3212.703	463.085	3124.358	-41.845
4000	1009.033	2563.707	1735.319	3313.553	460.594	3192.702	-41.692
4100	1010.052	2588.635	1755.829	3414.508	457.745	3261.040	-41.545
4200	1011.002	2612.987	1775.948	3515.561	454.564	3329.444	-41.407
4300	1011.890	2636.787	1795.692	3616.706	451.037	3397.842	-41.275
4400	1012.721	2660.059	1815.073	3717.937	447.174	3466.414	-41.151
4500	1013.499	2682.827	1834.105	3819.248	442.988	3535.133	-41.034
4600	1014.229	2705.110	1852.798	3920.635	438.428	3603.954	-40.923
4700	1014.915	2726.930	1871.166	4022.093	433.510	3672.769	-40.817
4800	1015.559	2748.304	1889.217	4123.617	428.278	3741.794	-40.718
4900	1016.167	2769.251	1906.964	4225.203	422.661	3810.802	-40.623
5000	1016.739	2789.786	1924.416	4326.849	416.748	3880.109	-40.534

3.296. Benzo[*a*]naphtho[1,2-*h*]anthracene



Other names: Dibenzo[*a,k*]tetraphene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 18429-26-0

Point Group: C₁

Length: 16.30 Å

Width: 10.15 Å

Breadth: 4.967 Å

L/B Ratio: 1.606

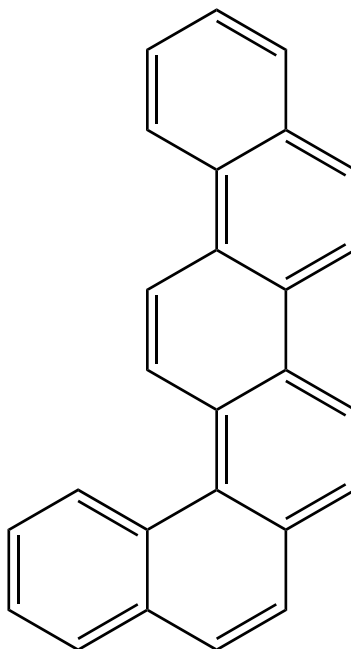
Cartesian coordinates:

C	-5.5933	1.2687	-0.1384	C	0.4501	-2.9109	0.1887	H	-6.4566	-1.9432	0.5607
C	-6.3916	0.1756	0.1266	C	1.7826	-3.0524	0.0065	H	-3.9731	-2.2118	0.4848
C	-5.8139	-1.0816	0.3526	C	2.1146	-0.6079	-0.0089	H	-1.3671	3.0102	-0.7112
C	-4.4440	-1.2318	0.3125	C	2.6306	-1.9022	-0.1199	H	-3.8363	3.2340	-0.6427
C	-4.1924	1.1312	-0.1823	C	4.0216	-2.1255	-0.3532	H	-2.1656	-2.3879	0.3453
C	-3.6115	-0.1278	0.0465	C	4.8857	-1.0814	-0.4232	H	0.6086	1.6635	-0.4920
C	-2.0065	2.1457	-0.4979	C	3.0584	0.4817	0.1121	H	-0.1995	-3.7808	0.3385
C	-3.3514	2.2678	-0.4613	C	4.4249	0.2423	-0.1519	H	2.2450	-4.0460	-0.0235
C	-1.3691	0.8747	-0.2550	C	5.3641	1.3014	-0.0970	H	4.3722	-3.1549	-0.4925
C	-2.1681	-0.2651	0.0032	C	4.9736	2.5601	0.2815	H	5.9467	-1.2373	-0.6493
C	-1.5413	-1.4940	0.1821	C	3.6328	2.7904	0.6406	H	6.4108	1.0951	-0.3488
C	0.0195	0.7619	-0.2691	C	2.7067	1.7808	0.5592	H	5.6952	3.3820	0.3244
C	0.6687	-0.4561	-0.0246	H	-6.0417	2.2526	-0.3172	H	3.3352	3.7836	0.9932
C	-0.1470	-1.6076	0.1372	H	-7.4806	0.2838	0.1610	H	1.6723	1.9853	0.8675

Table 3.296: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[1,2-*h*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.486	437.566	437.566	∞
100	108.882	351.160	778.148	-42.699	464.377	512.318	-267.602
200	213.436	456.854	591.123	-26.854	450.195	565.909	-147.797
250	274.598	510.999	569.657	-14.665	443.520	595.611	-124.444
298.15	334.393	564.488	564.488	0.000	437.566	625.458	-109.575
300	336.665	566.564	564.495	0.621	437.347	626.622	-109.102
350	396.460	622.996	568.815	18.963	431.852	658.615	-98.291
400	451.980	679.615	579.128	40.195	427.075	691.336	-90.277
450	502.319	735.809	593.421	64.075	422.939	724.621	-84.110
500	547.352	791.110	610.434	90.338	419.358	758.357	-79.223
600	622.962	897.860	649.521	149.003	413.563	826.732	-71.972
700	682.882	998.563	692.266	214.408	409.366	895.952	-66.855
800	731.057	1093.007	736.520	285.189	406.577	965.660	-63.050
900	770.417	1181.460	781.098	360.327	405.013	1035.637	-60.106
1000	803.011	1264.371	825.324	439.048	404.504	1105.743	-57.757
1100	830.286	1342.223	868.812	520.752	404.852	1175.865	-55.836
1200	853.303	1415.482	911.346	604.963	405.913	1245.906	-54.232
1300	872.861	1484.576	952.808	691.297	407.506	1315.847	-52.870
1400	889.580	1549.889	993.146	779.441	409.497	1385.654	-51.698
1500	903.953	1611.766	1032.343	869.135	411.804	1455.308	-50.677
1600	916.372	1670.512	1070.408	960.166	414.297	1524.792	-49.778
1700	927.157	1726.398	1107.366	1052.355	416.902	1594.093	-48.980
1800	936.567	1779.665	1143.248	1145.552	419.544	1663.302	-48.267
1900	944.814	1830.529	1178.092	1239.630	422.192	1732.313	-47.624
2000	952.073	1879.180	1211.939	1334.482	424.790	1801.211	-47.042
2100	958.490	1925.790	1244.830	1430.017	427.263	1869.967	-46.512
2200	964.184	1970.513	1276.806	1526.156	429.608	1938.612	-46.028
2300	969.256	2013.487	1307.907	1622.833	431.819	2007.152	-45.583
2400	973.791	2054.835	1338.173	1719.989	433.827	2075.553	-45.172
2500	977.859	2094.672	1367.641	1817.575	435.644	2143.985	-44.795
2600	981.520	2133.096	1396.347	1915.547	437.232	2212.235	-44.443
2700	984.825	2170.202	1424.325	2013.867	438.596	2280.497	-44.118
2800	987.818	2206.073	1451.608	2112.502	439.710	2348.736	-43.815
2900	990.536	2240.785	1478.226	2211.422	440.546	2416.887	-43.532
3000	993.011	2274.408	1504.208	2310.601	441.145	2485.039	-43.267
3100	995.270	2307.006	1529.581	2410.017	441.433	2553.103	-43.019
3200	997.337	2338.638	1554.373	2509.649	441.449	2621.232	-42.786
3300	999.233	2369.357	1578.606	2609.478	441.175	2689.402	-42.569
3400	1000.976	2399.213	1602.304	2709.490	440.584	2757.503	-42.363
3500	1002.582	2428.253	1625.490	2809.669	439.681	2825.608	-42.169
3600	1004.064	2456.517	1648.183	2910.002	438.487	2893.826	-41.987
3700	1005.435	2484.046	1670.404	3010.478	436.970	2962.100	-41.817
3800	1006.705	2510.877	1692.170	3111.086	435.106	3030.359	-41.654
3900	1007.884	2537.042	1713.499	3211.816	432.934	3098.624	-41.501
4000	1008.981	2562.573	1734.408	3312.660	430.438	3167.081	-41.357
4100	1010.002	2587.500	1754.913	3413.610	427.584	3235.533	-41.220
4200	1010.955	2611.850	1775.027	3514.658	424.398	3304.051	-41.091
4300	1011.845	2635.649	1794.766	3615.799	420.867	3372.562	-40.968
4400	1012.677	2658.921	1814.142	3717.025	416.999	3441.248	-40.852
4500	1013.457	2681.687	1833.169	3818.332	412.809	3510.081	-40.743
4600	1014.189	2703.970	1851.858	3919.715	408.245	3579.016	-40.640
4700	1014.876	2725.789	1870.221	4021.169	403.323	3647.945	-40.542
4800	1015.522	2747.162	1888.269	4122.689	398.087	3717.084	-40.449
4900	1016.131	2768.108	1906.012	4224.272	392.466	3786.206	-40.361
5000	1016.704	2788.642	1923.460	4325.914	386.550	3855.628	-40.279

3.297. Benzo[*a*]picene



Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 58029-45-1
Point Group: C₁

Length: 16.23 Å
Width: 9.985 Å
Breadth: 4.809 Å
L/B Ratio: 1.625

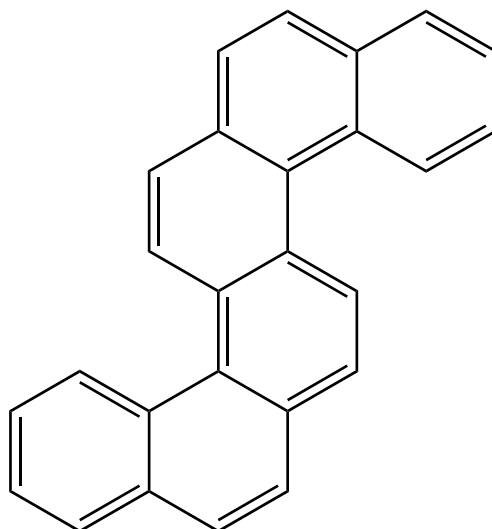
Cartesian coordinates:

C	5.3845	2.1485	-0.2798	C	-0.2380	-2.5768	0.1462	H	6.5090	-0.9978	0.4073
C	6.2837	1.0984	-0.0150	C	-1.5608	-2.8537	0.0051	H	3.3178	2.7191	-0.5304
C	5.8152	-0.1748	0.2017	C	-2.1070	-0.4588	-0.0436	H	4.6427	-2.5663	0.5826
C	4.0327	1.9085	-0.3219	C	-2.5108	-1.7992	-0.1137	H	2.2080	-3.0305	0.5117
C	3.5251	0.6070	-0.0996	C	-3.8843	-2.1496	-0.3133	H	-0.8634	1.9275	-0.6309
C	4.4265	-0.4402	0.1620	C	-4.8366	-1.1892	-0.3878	H	1.5577	2.3631	-0.6452
C	3.9250	-1.7622	0.3834	C	-3.1468	0.5451	0.0798	H	0.4950	-3.3845	0.2909
C	2.5917	-2.0125	0.3458	C	-4.4902	0.1788	-0.1513	H	-1.9185	-3.8900	-0.0010
C	2.1108	0.3298	-0.1330	C	-5.5197	1.1470	-0.0911	H	-4.1426	-3.2093	-0.4245
C	1.6446	-0.9676	0.0918	C	-5.2381	2.4433	0.2623	H	-5.8839	-1.4416	-0.5892
C	-0.1682	1.1112	-0.3918	C	-3.9189	2.7994	0.5895	H	-6.5484	0.8431	-0.3169
C	1.1701	1.3593	-0.4112	C	-2.9057	1.8750	0.5020	H	-6.0314	3.1961	0.3091
C	-0.6907	-0.1837	-0.0979	H	5.7727	3.1576	-0.4522	H	-3.7044	3.8206	0.9215
C	0.2321	-1.2342	0.0619	H	7.3582	1.3065	0.0157	H	-1.8882	2.1785	0.7834

Table 3.297: Table of thermodynamic data as a function of temperature for Benzo[*a*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.706	438.480	438.480	∞
100	109.720	353.450	781.781	-42.833	465.157	512.869	-267.890
200	214.109	459.683	594.239	-26.911	451.051	566.200	-147.873
250	275.181	513.968	572.731	-14.691	444.408	595.757	-124.474
298.15	334.900	567.554	567.554	0.000	438.480	625.458	-109.575
300	337.170	569.632	567.560	0.622	438.262	626.617	-109.101
350	396.903	626.137	571.886	18.988	432.790	658.454	-98.267
400	452.373	682.812	582.211	40.240	428.035	691.016	-90.236
450	502.670	739.050	596.520	64.139	423.917	724.141	-84.054
500	547.663	794.386	613.549	90.419	420.353	757.714	-79.156
600	623.194	901.185	652.667	149.111	414.585	825.758	-71.887
700	683.039	1001.919	695.440	214.535	410.408	894.645	-66.758
800	731.146	1096.379	739.718	285.328	407.631	964.016	-62.942
900	770.449	1184.839	784.315	360.472	406.072	1033.655	-59.991
1000	802.998	1267.751	828.557	439.194	405.564	1103.423	-57.636
1100	830.242	1345.600	872.059	520.895	405.909	1173.208	-55.710
1200	853.236	1418.854	914.604	605.101	406.965	1242.911	-54.101
1300	872.778	1487.942	956.075	691.427	408.550	1312.515	-52.736
1400	889.488	1553.249	996.419	779.562	410.532	1381.985	-51.561
1500	903.855	1615.120	1035.622	869.247	412.829	1451.304	-50.538
1600	916.273	1673.859	1073.691	960.268	415.313	1520.453	-49.637
1700	927.057	1729.739	1110.652	1052.447	417.907	1589.420	-48.836
1800	936.469	1783.000	1146.537	1145.634	420.540	1658.295	-48.121
1900	944.718	1833.858	1181.384	1239.702	423.178	1726.973	-47.477
2000	951.981	1882.505	1215.232	1334.545	425.767	1795.538	-46.894
2100	958.401	1929.111	1248.125	1430.070	428.231	1863.962	-46.363
2200	964.098	1973.829	1280.102	1526.201	430.567	1932.275	-45.877
2300	969.174	2016.799	1311.204	1622.869	432.770	2000.483	-45.431
2400	973.713	2058.145	1341.471	1720.018	434.770	2068.554	-45.020
2500	977.784	2097.978	1370.939	1817.596	436.578	2136.654	-44.642
2600	981.448	2136.400	1399.645	1915.561	438.159	2204.574	-44.290
2700	984.757	2173.503	1427.624	2013.874	439.516	2272.506	-43.963
2800	987.753	2209.371	1454.906	2112.502	440.624	2340.415	-43.660
2900	990.474	2244.081	1481.524	2211.415	441.454	2408.236	-43.376
3000	992.952	2277.702	1507.506	2310.589	442.047	2476.059	-43.111
3100	995.214	2310.298	1532.879	2409.999	442.329	2543.793	-42.862
3200	997.283	2341.928	1557.670	2509.625	442.339	2611.593	-42.629
3300	999.182	2372.646	1581.903	2609.450	442.060	2679.435	-42.411
3400	1000.927	2402.501	1605.602	2709.456	441.465	2747.207	-42.205
3500	1002.535	2431.538	1628.787	2809.630	440.557	2814.983	-42.010
3600	1004.020	2459.802	1651.480	2909.959	439.358	2882.873	-41.829
3700	1005.392	2487.330	1673.700	3010.431	437.837	2950.818	-41.657
3800	1006.665	2514.159	1695.466	3111.034	435.969	3018.749	-41.495
3900	1007.845	2540.323	1716.795	3211.761	433.793	3086.686	-41.341
4000	1008.944	2565.854	1737.703	3312.601	431.293	3154.815	-41.197
4100	1009.966	2590.780	1758.207	3413.547	428.435	3222.939	-41.060
4200	1010.920	2615.129	1778.321	3514.592	425.246	3291.129	-40.930
4300	1011.812	2638.927	1798.060	3615.729	421.711	3359.312	-40.807
4400	1012.645	2662.198	1817.436	3716.952	417.840	3427.670	-40.691
4500	1013.427	2684.964	1836.462	3818.256	413.646	3496.175	-40.582
4600	1014.159	2707.246	1855.151	3919.636	409.080	3564.782	-40.479
4700	1014.848	2729.064	1873.514	4021.086	404.155	3633.384	-40.380
4800	1015.495	2750.437	1891.561	4122.604	398.916	3702.196	-40.287
4900	1016.105	2771.382	1909.303	4224.184	393.293	3770.991	-40.198
5000	1016.679	2791.916	1926.751	4325.824	387.374	3840.085	-40.116

3.298. Dibenzo[*c,l*]chrysene



Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 42850-69-1
Point Group: C_{2h}

Length: 15.73 Å
Width: 9.358 Å
Breadth: 4.686 Å
L/B Ratio: 1.680

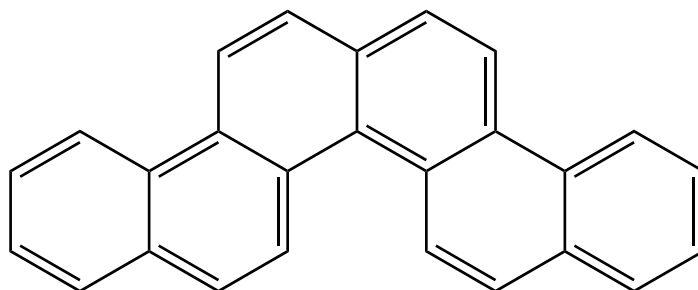
Cartesian coordinates:

C	-3.4355	-1.5524	0.3510	C	0.5508	-2.4279	-0.4144	H	-6.8100	-1.7006	-0.0304
C	-4.7062	-2.0769	0.3320	C	-0.5984	-1.7035	-0.4603	H	-6.4641	0.7322	-0.4268
C	-5.8068	-1.2649	0.0128	C	1.7909	-1.7963	-0.1257	H	-5.0538	2.6668	-0.4374
C	-5.6124	0.0751	-0.2158	C	1.8612	-0.4010	-0.0226	H	-2.8288	3.7062	-0.0238
C	-3.1867	-0.1926	0.0461	C	4.1658	-2.0534	0.2473	H	-0.5436	3.5035	0.6313
C	-4.3138	0.6322	-0.1615	C	2.9516	-2.6170	0.0425	H	1.5285	2.1966	0.7752
C	-4.1657	2.0534	-0.2478	C	4.3140	-0.6323	0.1594	H	0.5430	-3.5036	-0.6264
C	-2.9520	2.6171	-0.0402	C	3.1867	0.1927	-0.0457	H	-1.5288	-2.1964	-0.7727
C	-1.8613	0.4014	0.0248	C	3.4355	1.5527	-0.3503	H	5.0542	-2.6669	0.4358
C	-1.7913	1.7966	0.1288	C	4.7063	2.0766	-0.3344	H	2.8280	-3.7060	0.0279
C	-0.5514	2.4280	0.4181	C	5.8076	1.2640	-0.0189	H	2.5993	2.2088	-0.6269
C	0.5979	1.7039	0.4630	C	5.6131	-0.0758	0.2101	H	4.8686	3.1325	-0.5752
C	-0.6193	-0.3252	-0.0971	H	-2.6000	-2.2079	0.6308	H	6.8110	1.6994	0.0212
C	0.6192	0.3256	0.0993	H	-4.8688	-3.1327	0.5728	H	6.4650	-0.7333	0.4191

Table 3.298: Table of thermodynamic data as a function of temperature for Dibenzo[*c,l*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.418	471.642	471.642	∞
100	108.167	344.642	771.301	-42.666	498.486	547.079	-285.759
200	213.307	450.022	584.335	-26.863	484.262	601.343	-157.051
250	274.700	504.163	562.860	-14.674	477.586	631.386	-131.918
298.15	334.681	557.687	557.687	0.000	471.642	661.562	-115.900
300	336.960	559.764	557.693	0.621	471.424	662.739	-115.391
350	396.910	616.254	562.018	18.983	465.947	695.070	-103.731
400	452.542	672.941	572.342	40.240	461.196	728.126	-95.082
450	502.951	729.206	586.651	64.149	457.090	761.743	-88.419
500	548.015	784.575	603.684	90.445	453.542	795.808	-83.136
600	623.606	891.445	642.818	149.176	447.813	864.830	-75.289
700	683.447	992.242	685.611	214.642	443.676	934.687	-69.746
800	731.525	1086.755	729.911	285.475	440.939	1005.023	-65.620
900	770.791	1175.258	774.531	360.654	439.417	1075.623	-62.426
1000	803.303	1258.204	818.796	439.409	438.941	1146.347	-59.878
1100	830.511	1336.081	862.318	521.139	439.315	1217.085	-57.793
1200	853.474	1409.357	904.882	605.370	440.396	1287.739	-56.053
1300	872.989	1478.462	946.371	691.719	442.003	1358.292	-54.576
1400	889.676	1543.784	986.732	779.873	444.006	1428.709	-53.305
1500	904.023	1605.667	1025.950	869.576	446.320	1498.974	-52.198
1600	916.423	1664.417	1064.034	960.613	448.820	1569.068	-51.224
1700	927.193	1720.305	1101.008	1052.806	451.429	1638.978	-50.359
1800	936.591	1773.574	1136.904	1146.006	454.074	1708.796	-49.587
1900	944.829	1824.439	1171.762	1240.086	456.724	1778.416	-48.891
2000	952.082	1873.090	1205.621	1334.939	459.324	1847.923	-48.262
2100	958.493	1919.701	1238.523	1430.474	461.797	1917.288	-47.689
2200	964.183	1964.424	1270.509	1526.614	464.142	1986.542	-47.166
2300	969.252	2007.398	1301.619	1623.290	466.353	2055.690	-46.685
2400	973.785	2048.746	1331.893	1720.446	468.361	2124.701	-46.242
2500	977.851	2088.582	1361.369	1818.032	470.176	2193.741	-45.835
2600	981.510	2127.006	1390.082	1916.003	471.763	2262.601	-45.455
2700	984.815	2164.112	1418.067	2014.322	473.126	2331.472	-45.104
2800	987.807	2199.982	1445.355	2112.956	474.240	2400.320	-44.778
2900	990.524	2234.694	1471.979	2211.874	475.075	2469.080	-44.472
3000	992.999	2268.317	1497.966	2311.052	475.673	2537.841	-44.187
3100	995.258	2300.914	1523.344	2410.467	475.959	2606.514	-43.919
3200	997.325	2332.545	1548.140	2510.098	475.974	2675.252	-43.668
3300	999.221	2363.264	1572.378	2609.926	475.698	2744.032	-43.434
3400	1000.964	2393.120	1596.080	2709.937	475.107	2812.742	-43.212
3500	1002.570	2422.159	1619.269	2810.114	474.203	2881.457	-43.002
3600	1004.053	2450.424	1641.966	2910.447	473.007	2950.284	-42.807
3700	1005.424	2477.952	1664.190	3010.921	471.490	3019.167	-42.622
3800	1006.694	2504.782	1685.959	3111.528	469.624	3088.035	-42.447
3900	1007.874	2530.947	1707.292	3212.257	467.451	3156.910	-42.281
4000	1008.970	2556.478	1728.203	3313.100	464.954	3225.977	-42.126
4100	1009.992	2581.405	1748.710	3414.049	462.099	3295.038	-41.978
4200	1010.945	2605.755	1768.827	3515.096	458.912	3364.165	-41.839
4300	1011.835	2629.554	1788.569	3616.235	455.380	3433.286	-41.705
4400	1012.668	2652.825	1807.947	3717.461	451.511	3502.582	-41.580
4500	1013.448	2675.591	1826.976	3818.767	447.320	3572.024	-41.462
4600	1014.180	2697.874	1845.668	3920.149	442.755	3641.568	-41.350
4700	1014.867	2719.692	1864.033	4021.602	437.832	3711.107	-41.243
4800	1015.514	2741.066	1882.082	4123.121	432.595	3780.856	-41.143
4900	1016.123	2762.011	1899.827	4224.703	426.974	3850.588	-41.047
5000	1016.696	2782.545	1917.277	4326.344	421.057	3920.619	-40.958

3.299. Naphtho[1,2-*c*]chrysene



Formula: $C_{26}H_{16}$
Mass: 328.405 g/mol
CAS Number: 58029-46-2
Point Group: C_2

Length: 16.77 Å
Width: 9.380 Å
Breadth: 4.957 Å
L/B Ratio: 1.788

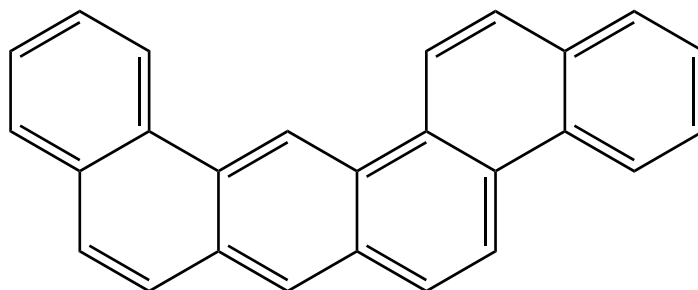
Cartesian coordinates:

C	6.1548	-0.1090	0.2962	C	-2.4034	-2.1441	-0.2289	H	5.0964	3.0311	-0.5095
C	6.2138	1.2660	-0.0001	C	-1.2155	-2.7975	-0.1391	H	4.8958	-1.8389	0.5426
C	5.0618	1.9612	-0.2748	C	-2.4608	-0.7300	-0.0687	H	2.6730	3.0568	-0.8585
C	4.9476	-0.7634	0.3155	C	-1.2781	0.0028	0.1095	H	0.4923	1.9420	-0.7413
C	3.7438	-0.0694	0.0441	C	-1.4011	1.3808	0.4846	H	1.1712	-3.8917	0.1904
C	3.8106	1.3016	-0.2570	C	-2.6043	2.0045	0.5591	H	3.3440	-2.6929	0.3885
C	2.6042	2.0045	-0.5591	C	-3.7438	-0.0695	-0.0441	H	-3.3441	-2.6926	-0.3885
C	1.4011	1.3806	-0.4844	C	-3.8106	1.3015	0.2570	H	-1.1712	-3.8917	-0.1904
C	2.4608	-0.7300	0.0687	C	-5.0617	1.9612	0.2748	H	-0.4916	1.9411	0.7413
C	1.2781	0.0027	-0.1095	C	-6.2138	1.2660	-0.0000	H	-2.6730	3.0567	0.8586
C	1.2155	-2.7975	0.1391	C	-6.1548	-0.1090	-0.2963	H	-5.0963	3.0311	0.5095
C	2.4034	-2.1441	0.2289	C	-4.9477	-0.7634	-0.3156	H	-7.1843	1.7726	0.0100
C	0.0000	-2.0673	0.0000	H	7.0810	-0.6519	0.5111	H	-7.0810	-0.6519	-0.5112
C	-0.0000	-0.6614	0.0000	H	7.1843	1.7726	-0.0101	H	-4.8954	-1.8389	-0.5426

Table 3.299: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*c*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.686	439.633	439.633	∞
100	109.602	346.744	775.003	-42.826	466.317	514.700	-268.846
200	214.082	452.918	587.478	-26.912	452.203	568.705	-148.527
250	275.192	507.202	565.969	-14.692	445.559	598.600	-125.068
298.15	334.931	560.791	560.791	0.000	439.633	628.627	-110.131
300	337.201	562.869	560.797	0.622	439.415	629.799	-109.655
350	396.941	619.380	565.123	18.990	433.945	661.974	-98.792
400	452.412	676.060	575.450	40.244	429.191	694.874	-90.739
450	502.706	732.303	589.760	64.144	425.075	728.336	-84.541
500	547.696	787.642	606.790	90.426	421.513	762.246	-79.630
600	623.223	894.447	645.911	149.121	415.748	830.965	-72.340
700	683.065	995.185	688.687	214.548	411.573	900.524	-67.197
800	731.172	1089.648	732.968	285.344	408.799	970.569	-63.370
900	770.476	1178.112	777.567	360.490	407.243	1040.881	-60.410
1000	803.026	1261.027	821.812	439.215	406.738	1111.322	-58.048
1100	830.269	1338.878	865.315	520.919	407.086	1181.778	-56.117
1200	853.263	1412.135	907.862	605.128	408.145	1252.154	-54.504
1300	872.805	1481.225	949.335	691.457	409.732	1322.430	-53.135
1400	889.514	1546.534	989.681	779.594	411.717	1392.572	-51.956
1500	903.880	1608.406	1028.885	869.282	414.017	1462.562	-50.930
1600	916.296	1667.147	1066.956	960.305	416.502	1532.382	-50.026
1700	927.080	1723.028	1103.918	1052.487	419.100	1602.020	-49.223
1800	936.490	1776.291	1139.805	1145.676	421.735	1671.566	-48.507
1900	944.738	1827.150	1174.652	1239.746	424.375	1740.915	-47.860
2000	952.000	1875.797	1208.502	1334.590	426.965	1810.150	-47.275
2100	958.419	1922.404	1241.396	1430.118	429.431	1879.245	-46.743
2200	964.115	1967.124	1273.374	1526.250	431.769	1948.229	-46.256
2300	969.190	2010.095	1304.477	1622.920	433.973	2017.108	-45.809
2400	973.728	2051.441	1334.745	1720.070	435.975	2085.849	-45.396
2500	977.798	2091.274	1364.214	1817.650	437.785	2154.620	-45.017
2600	981.462	2129.697	1392.921	1915.616	439.367	2223.210	-44.664
2700	984.770	2166.800	1420.900	2013.931	440.726	2291.812	-44.337
2800	987.765	2202.669	1448.184	2112.560	441.835	2360.391	-44.033
2900	990.486	2237.379	1474.802	2211.475	442.666	2428.883	-43.748
3000	992.963	2271.001	1500.785	2310.649	443.260	2497.375	-43.482
3100	995.224	2303.597	1526.159	2410.060	443.543	2565.780	-43.232
3200	997.293	2335.228	1550.950	2509.687	443.554	2634.250	-42.999
3300	999.191	2365.945	1575.184	2609.513	443.276	2702.761	-42.780
3400	1000.936	2395.801	1598.883	2709.520	442.681	2771.204	-42.573
3500	1002.544	2424.839	1622.069	2809.696	441.775	2839.650	-42.379
3600	1004.028	2453.102	1644.762	2910.025	440.576	2908.209	-42.196
3700	1005.400	2480.631	1666.983	3010.497	439.056	2976.825	-42.024
3800	1006.672	2507.460	1688.749	3111.102	437.189	3045.425	-41.861
3900	1007.852	2533.624	1710.078	3211.829	435.014	3114.032	-41.707
4000	1008.950	2559.155	1730.987	3312.669	432.514	3182.831	-41.563
4100	1009.973	2584.081	1751.492	3413.616	429.657	3251.625	-41.425
4200	1010.926	2608.431	1771.606	3514.662	426.469	3320.485	-41.295
4300	1011.817	2632.229	1791.345	3615.799	422.934	3389.338	-41.171
4400	1012.651	2655.500	1810.722	3717.023	419.064	3458.366	-41.055
4500	1013.432	2678.266	1829.748	3818.328	414.871	3527.541	-40.946
4600	1014.165	2700.548	1848.437	3919.708	410.305	3596.818	-40.842
4700	1014.853	2722.366	1866.800	4021.159	405.380	3666.089	-40.743
4800	1015.500	2743.739	1884.848	4122.677	400.142	3735.571	-40.650
4900	1016.109	2764.684	1902.591	4224.258	394.519	3805.035	-40.561
5000	1016.684	2785.218	1920.039	4325.898	388.601	3874.800	-40.479

3.300. Naphtho[2,1-*b*]chrysene



Other names: Dibenzo[*c,m*]tetraphene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 58029-43-9

Point Group: C_s

Length: 16.62 Å

Width: 9.513 Å

Breadth: 3.885 Å

L/B Ratio: 1.747

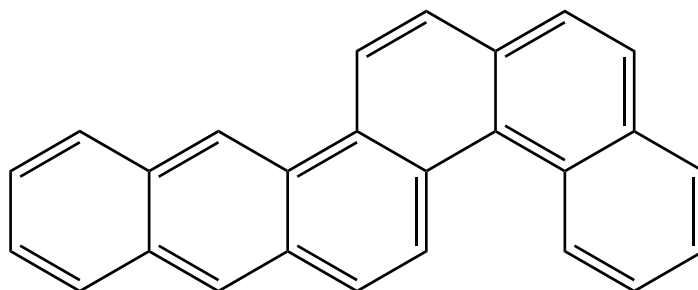
Cartesian coordinates:

C	5.8299	-2.1081	0.0000	C	-1.2043	2.6566	0.0000	H	2.4322	-2.4635	0.0000
C	5.9136	-0.7314	0.0000	C	-2.4330	2.0858	0.0000	H	4.5212	-3.8311	0.0000
C	3.4232	-1.9838	0.0000	C	-1.4619	-0.1577	0.0000	H	5.8208	1.9493	0.0000
C	4.5775	-2.7378	0.0000	C	-2.5905	0.6601	0.0000	H	3.7693	3.3447	0.0000
C	3.4866	-0.5772	0.0000	C	-2.8519	-2.1477	0.0000	H	1.3401	3.5277	0.0000
C	4.7433	0.0518	0.0000	C	-1.6179	-1.5773	0.0000	H	0.9272	-1.4508	0.0000
C	4.8252	1.4907	0.0000	C	-4.0262	-1.3346	0.0000	H	-1.0890	3.7466	0.0000
C	3.7085	2.2502	0.0000	C	-3.9018	0.0675	0.0000	H	-3.3469	2.6997	0.0000
C	2.2817	0.2325	0.0000	C	-5.0781	0.8574	0.0000	H	-2.9678	-3.2376	0.0000
C	2.3989	1.6461	0.0000	C	-6.3172	0.2686	0.0000	H	-0.7059	-2.1942	0.0000
C	1.2510	2.4341	0.0000	C	-6.4373	-1.1356	0.0000	H	-4.9715	1.9528	0.0000
C	1.0167	-0.3475	0.0000	C	-5.3142	-1.9240	0.0000	H	-7.2226	0.8842	0.0000
C	-0.1437	0.4362	0.0000	H	6.7406	-2.7159	0.0000	H	-7.4340	-1.5887	0.0000
C	-0.0201	1.8459	0.0000	H	6.8910	-0.2355	0.0000	H	-5.3985	-3.0167	0.0000

Table 3.300: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-50.080	414.837	414.837	∞
100	111.331	358.331	788.701	-43.037	441.310	488.534	-255.179
200	215.062	465.435	600.402	-26.993	427.326	541.325	-141.377
250	276.011	519.918	578.833	-14.729	420.727	570.588	-119.215
298.15	335.644	573.642	573.642	0.000	414.837	600.000	-105.115
300	337.911	575.725	573.649	0.623	414.621	601.148	-104.667
350	397.555	632.338	577.983	19.024	409.184	632.678	-94.420
400	452.938	689.094	588.327	40.307	404.458	664.927	-86.829
450	503.154	745.394	602.658	64.231	400.367	697.736	-80.989
500	548.078	800.777	619.710	90.534	396.825	730.991	-76.364
600	623.511	907.642	658.872	149.262	391.094	798.392	-69.505
700	683.300	1008.421	701.685	214.715	386.945	866.630	-64.667
800	731.379	1102.913	745.997	285.533	384.192	935.350	-61.071
900	770.667	1191.400	790.624	360.699	382.656	1004.335	-58.289
1000	803.206	1274.335	834.893	439.442	382.170	1073.445	-56.070
1100	830.442	1352.203	878.418	521.164	382.535	1142.570	-54.255
1200	853.427	1425.474	920.983	605.389	383.610	1211.613	-52.739
1300	872.961	1494.577	962.473	691.734	385.214	1280.554	-51.452
1400	889.662	1559.897	1002.835	779.887	387.214	1349.360	-50.344
1500	904.020	1621.779	1042.054	869.589	389.528	1418.013	-49.379
1600	916.429	1680.529	1080.138	960.626	392.028	1486.496	-48.528
1700	927.205	1736.418	1117.112	1052.820	394.638	1554.795	-47.772
1800	936.607	1789.688	1153.010	1146.021	397.285	1623.002	-47.097
1900	944.848	1840.553	1187.868	1240.103	399.936	1691.010	-46.488
2000	952.103	1889.206	1221.727	1334.958	402.538	1758.905	-45.937
2100	958.516	1935.818	1254.629	1430.496	405.013	1826.659	-45.435
2200	964.207	1980.542	1286.616	1526.637	407.361	1894.302	-44.976
2300	969.276	2023.516	1317.727	1623.316	409.574	1961.838	-44.554
2400	973.808	2064.866	1348.002	1720.475	411.584	2029.237	-44.164
2500	977.874	2104.703	1377.478	1818.062	413.402	2096.665	-43.807
2600	981.534	2143.128	1406.191	1916.036	414.991	2163.912	-43.473
2700	984.838	2180.235	1434.176	2014.357	416.357	2231.171	-43.164
2800	987.829	2216.106	1461.465	2112.993	417.472	2298.407	-42.876
2900	990.546	2250.818	1488.089	2211.914	418.309	2365.555	-42.607
3000	993.020	2284.442	1514.077	2311.094	418.910	2432.703	-42.356
3100	995.278	2317.040	1539.456	2410.511	419.198	2499.764	-42.120
3200	997.344	2348.672	1564.252	2510.143	419.215	2566.889	-41.899
3300	999.240	2379.391	1588.490	2609.974	418.941	2634.056	-41.693
3400	1000.982	2409.248	1612.193	2709.986	418.352	2701.154	-41.497
3500	1002.588	2438.287	1635.383	2810.166	417.449	2768.255	-41.313
3600	1004.070	2466.552	1658.080	2910.500	416.255	2835.470	-41.141
3700	1005.440	2494.081	1680.304	3010.976	414.739	2902.740	-40.979
3800	1006.710	2520.912	1702.074	3111.584	412.876	2969.996	-40.825
3900	1007.889	2547.077	1723.406	3212.315	410.704	3037.257	-40.679
4000	1008.985	2572.608	1744.319	3313.159	408.209	3104.711	-40.543
4100	1010.006	2597.536	1764.826	3414.109	405.355	3172.159	-40.413
4200	1010.958	2621.886	1784.943	3515.158	402.170	3239.674	-40.290
4300	1011.848	2645.685	1804.685	3616.299	398.639	3307.181	-40.173
4400	1012.680	2668.956	1824.064	3717.526	394.771	3374.864	-40.064
4500	1013.460	2691.723	1843.093	3818.833	390.581	3442.693	-39.961
4600	1014.192	2714.006	1861.785	3920.216	386.018	3510.624	-39.864
4700	1014.879	2735.825	1880.150	4021.670	381.096	3578.550	-39.770
4800	1015.525	2757.198	1898.200	4123.191	375.860	3646.685	-39.683
4900	1016.133	2778.144	1915.945	4224.774	370.239	3714.804	-39.599
5000	1016.707	2798.678	1933.395	4326.416	364.324	3783.222	-39.522

3.301. Dibenzo[*b,l*]chrysene



Other names: Naphtho[2,1-*c*]tetraphene
Phenanthro[3,4-*a*]anthracene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 58029-38-2
Point Group: C₁

Length: 16.79 Å
Width: 9.369 Å
Breadth: 4.944 Å
L/B Ratio: 1.793

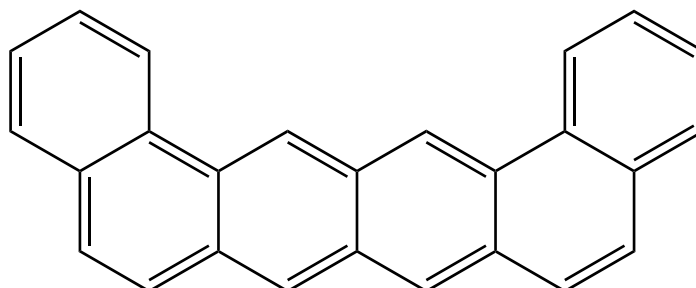
Cartesian coordinates:

C	6.4444	-0.7920	0.3879	C	-1.1597	-2.6891	-0.0086	H	5.7001	2.4792	-0.2818
C	6.6331	0.5955	0.1415	C	0.0957	-2.1603	0.0645	H	5.0378	-2.3981	0.5849
C	5.5647	1.4087	-0.0910	C	-2.2912	-1.8384	-0.0902	H	3.2653	2.7627	-0.5239
C	5.1924	-1.3298	0.3957	C	-2.1444	-0.4408	-0.0564	H	2.6073	-2.1144	0.3495
C	4.0497	-0.5053	0.1560	C	-4.7006	-1.6816	-0.2750	H	0.8564	3.0260	-0.8543
C	4.2381	0.8768	-0.0903	C	-3.5838	-2.4438	-0.2273	H	-1.4159	2.1201	-0.7379
C	3.1212	1.6928	-0.3295	C	-4.6100	-0.2662	-0.0712	H	-1.3096	-3.7750	0.0082
C	2.7512	-1.0385	0.1613	C	-3.3528	0.3513	0.0991	H	0.9769	-2.8096	0.1797
C	1.6433	-0.2302	-0.0676	C	-3.3509	1.7089	0.4968	H	-5.6890	-2.1295	-0.4290
C	1.8404	1.1547	-0.3209	C	-4.5174	2.4278	0.6165	H	-3.6413	-3.5351	-0.3139
C	0.6901	1.9770	-0.5824	C	-5.7560	1.8234	0.3498	H	-2.3988	2.2041	0.7305
C	-0.5601	1.4705	-0.5083	C	-5.8003	0.4898	0.0223	H	-4.4862	3.4774	0.9273
C	0.2906	-0.7611	-0.0496	H	7.3233	-1.4189	0.5709	H	-6.6755	2.4128	0.4215
C	-0.8153	0.0914	-0.1750	H	7.6518	0.9971	0.1423	H	-6.7612	-0.0067	-0.1560

Table 3.301: Table of thermodynamic data as a function of temperature for Dibenzo[*b,l*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.561	448.015	448.015	∞
100	108.880	350.865	778.770	-42.791	474.734	522.705	-273.027
200	213.944	456.742	591.323	-26.916	460.581	576.318	-150.516
250	275.247	511.017	569.808	-14.698	453.935	606.022	-126.619
298.15	335.114	564.627	564.627	0.000	448.015	635.865	-111.399
300	337.387	566.707	564.634	0.622	447.797	637.029	-110.914
350	397.199	623.253	568.963	19.001	442.338	669.012	-99.843
400	452.699	679.969	579.296	40.269	437.598	701.717	-91.633
450	503.000	736.246	593.615	64.184	433.497	734.983	-85.313
500	547.984	791.617	610.655	90.481	429.949	768.695	-80.303
600	623.495	898.472	649.799	149.204	424.213	837.014	-72.867
700	683.326	999.251	692.598	214.657	420.064	906.169	-67.618
800	731.427	1093.749	736.900	285.479	417.316	975.805	-63.712
900	770.727	1182.243	781.520	360.651	415.785	1045.706	-60.690
1000	803.272	1265.183	825.783	439.400	415.305	1115.731	-58.279
1100	830.510	1343.058	869.305	521.128	415.677	1185.772	-56.306
1200	853.495	1416.335	911.868	605.360	416.759	1255.728	-54.659
1300	873.027	1485.443	953.357	691.713	418.369	1325.583	-53.261
1400	889.725	1550.769	993.718	779.872	420.376	1395.302	-52.058
1500	904.080	1612.655	1032.935	869.580	422.696	1464.868	-51.010
1600	916.485	1671.409	1071.019	960.623	425.202	1534.263	-50.088
1700	927.258	1727.301	1107.994	1052.822	427.817	1603.474	-49.268
1800	936.657	1780.574	1143.891	1146.029	430.469	1672.592	-48.536
1900	944.896	1831.442	1178.750	1240.115	433.126	1741.512	-47.877
2000	952.147	1880.097	1212.609	1334.975	435.732	1810.318	-47.280
2100	958.557	1926.710	1245.512	1430.517	438.211	1878.983	-46.736
2200	964.246	1971.436	1277.499	1526.662	440.563	1947.536	-46.239
2300	969.313	2014.413	1308.611	1623.345	442.780	2015.983	-45.783
2400	973.843	2055.764	1338.886	1720.507	444.794	2084.292	-45.362
2500	977.907	2095.602	1368.363	1818.098	446.615	2152.630	-44.976
2600	981.564	2134.029	1397.077	1916.075	448.208	2220.787	-44.615
2700	984.866	2171.136	1425.062	2014.399	449.576	2288.956	-44.282
2800	987.856	2207.008	1452.352	2113.038	450.694	2357.102	-43.971
2900	990.572	2241.722	1478.976	2211.961	451.534	2425.159	-43.681
3000	993.044	2275.346	1504.965	2311.144	452.137	2493.217	-43.410
3100	995.301	2307.945	1530.344	2410.563	452.428	2561.187	-43.155
3200	997.366	2339.577	1555.141	2510.198	452.446	2629.222	-42.917
3300	999.260	2370.298	1579.379	2610.030	452.175	2697.299	-42.694
3400	1001.002	2400.155	1603.083	2710.045	451.587	2765.306	-42.483
3500	1002.606	2429.195	1626.273	2810.226	450.687	2833.317	-42.284
3600	1004.087	2457.460	1648.971	2910.562	449.495	2901.440	-42.098
3700	1005.457	2484.990	1671.195	3011.040	447.981	2969.620	-41.923
3800	1006.726	2511.821	1692.966	3111.650	446.119	3037.784	-41.756
3900	1007.904	2537.986	1714.299	3212.382	443.949	3105.955	-41.599
4000	1009.000	2563.518	1735.211	3313.228	441.455	3174.318	-41.451
4100	1010.020	2588.446	1755.719	3414.179	438.602	3242.675	-41.311
4200	1010.972	2612.796	1775.837	3515.230	435.418	3311.098	-41.179
4300	1011.861	2636.596	1795.579	3616.372	431.889	3379.515	-41.052
4400	1012.693	2659.867	1814.958	3717.600	428.023	3448.106	-40.933
4500	1013.472	2682.634	1833.988	3818.908	423.833	3516.844	-40.822
4600	1014.203	2704.917	1852.680	3920.293	419.271	3585.684	-40.716
4700	1014.890	2726.736	1871.045	4021.748	414.350	3654.519	-40.615
4800	1015.535	2748.110	1889.096	4123.269	409.116	3723.563	-40.520
4900	1016.143	2769.056	1906.841	4224.853	403.496	3792.591	-40.429
5000	1016.716	2789.591	1924.291	4326.497	397.581	3861.918	-40.344

3.302. Dibenzo[*a,l*]naphthacene



Other names: 1,2,9,10-Dibenzotetracene
2',3'-Phenanthra-2,3-phenanthrene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 226-86-8
Point Group: C_{2v}

Length: 16.67 Å
Width: 9.496 Å
Breadth: 3.884 Å
L/B Ratio: 1.755

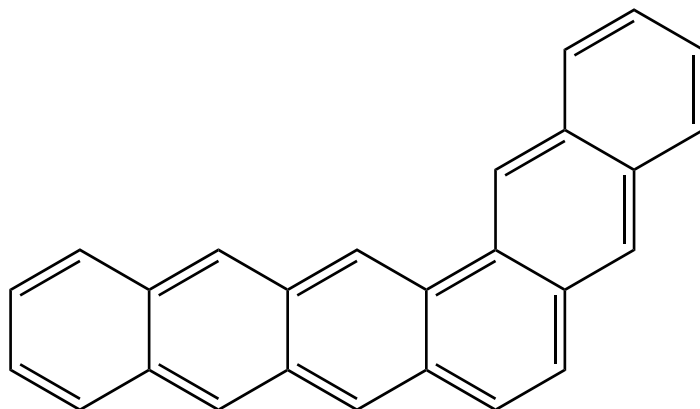
Cartesian coordinates:

C	6.1747	-1.9329	0.0000	C	-1.2345	2.2073	0.0000	H	2.8220	-2.5808	0.0000
C	6.1377	-0.5522	0.0000	C	-1.2319	-0.5954	0.0000	H	5.0208	-3.7619	0.0000
C	3.7666	-2.0155	0.0000	C	-2.4324	0.0873	0.0000	H	5.8171	2.1082	0.0000
C	4.9836	-2.6677	0.0000	C	-2.4307	1.5169	0.0000	H	3.6571	3.3253	0.0000
C	3.7078	-0.6107	0.0000	C	-3.6912	2.2250	0.0000	H	1.2258	3.3059	0.0000
C	4.9052	0.1244	0.0000	C	-4.8652	1.5621	0.0000	H	1.2395	-1.6960	0.0000
C	4.8633	1.5680	0.0000	C	-3.7070	-0.6151	0.0000	H	-1.2297	3.3045	0.0000
C	3.6885	2.2294	0.0000	C	-4.9054	0.1185	0.0000	H	-1.2376	-1.6974	0.0000
C	2.4322	0.0902	0.0000	C	-6.1370	-0.5596	0.0000	H	-3.6612	3.3209	0.0000
C	2.4289	1.5197	0.0000	C	-6.1723	-1.9404	0.0000	H	-5.8197	2.1011	0.0000
C	1.2318	2.2088	0.0000	C	-4.9803	-2.6737	0.0000	H	-7.0688	0.0175	0.0000
C	1.2325	-0.5940	0.0000	C	-3.7641	-2.0200	0.0000	H	-7.1325	-2.4665	0.0000
C	-0.0001	0.0980	0.0000	H	7.1356	-2.4578	0.0000	H	-5.0160	-3.7680	0.0000
C	-0.0009	1.5157	0.0000	H	7.0687	0.0261	0.0000	H	-2.8187	-2.5841	0.0000

Table 3.302: Table of thermodynamic data as a function of temperature for Dibenzo[*a,l*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.714	426.207	426.207	∞
100	109.768	348.464	776.776	-42.831	452.886	501.097	-261.741
200	214.120	454.701	589.246	-26.909	438.781	554.926	-144.929
250	275.167	508.987	567.740	-14.688	432.137	584.731	-122.170
298.15	334.800	562.563	562.563	0.000	426.207	614.673	-107.686
300	337.065	564.641	562.570	0.621	425.989	615.841	-107.225
350	396.670	621.121	566.894	18.979	420.509	647.929	-96.696
400	452.017	677.756	577.214	40.217	415.738	680.742	-88.894
450	502.220	733.947	591.514	64.095	411.600	714.121	-82.891
500	547.156	789.232	608.530	90.351	408.012	747.950	-78.136
600	622.673	895.936	647.618	148.991	402.192	816.515	-71.082
700	682.585	996.593	690.356	214.366	397.965	885.930	-66.108
800	730.791	1090.999	734.601	285.119	395.148	955.837	-62.408
900	770.195	1179.424	779.166	360.232	393.559	1026.016	-59.547
1000	802.833	1262.313	823.381	438.933	393.030	1096.327	-57.265
1100	830.148	1340.150	866.858	520.621	393.363	1166.656	-55.399
1200	853.197	1413.399	909.382	604.820	394.412	1236.905	-53.840
1300	872.780	1482.485	950.835	691.145	395.995	1307.054	-52.517
1400	889.521	1547.793	991.164	779.282	397.979	1377.070	-51.378
1500	903.909	1609.667	1030.353	868.971	400.281	1446.934	-50.386
1600	916.342	1668.410	1068.411	959.999	402.770	1516.629	-49.512
1700	927.136	1724.295	1105.362	1052.185	405.372	1586.140	-48.735
1800	936.553	1777.561	1141.239	1145.380	408.013	1655.559	-48.042
1900	944.806	1828.424	1176.078	1239.457	410.660	1724.781	-47.417
2000	952.070	1877.075	1209.920	1334.308	413.258	1793.889	-46.851
2100	958.490	1923.685	1242.807	1429.843	415.730	1862.856	-46.335
2200	964.187	1968.408	1274.780	1525.982	418.076	1931.711	-45.864
2300	969.261	2011.382	1305.878	1622.659	420.287	2000.461	-45.431
2400	973.797	2052.731	1336.140	1719.816	422.296	2069.074	-45.031
2500	977.866	2092.567	1365.606	1817.403	424.113	2137.715	-44.664
2600	981.528	2130.992	1394.309	1915.376	425.702	2206.176	-44.322
2700	984.834	2168.098	1422.285	2013.697	427.066	2274.648	-44.005
2800	987.827	2203.969	1449.565	2112.332	428.182	2343.098	-43.710
2900	990.545	2238.682	1476.181	2211.253	429.019	2411.459	-43.434
3000	993.020	2272.305	1502.161	2310.433	429.619	2479.821	-43.177
3100	995.279	2304.903	1527.533	2409.850	429.907	2548.096	-42.934
3200	997.346	2336.535	1552.322	2509.483	429.924	2616.435	-42.708
3300	999.242	2367.255	1576.554	2609.313	429.651	2684.815	-42.496
3400	1000.985	2397.111	1600.251	2709.326	429.062	2753.127	-42.296
3500	1002.591	2426.151	1623.435	2809.506	428.159	2821.442	-42.107
3600	1004.073	2454.416	1646.127	2909.840	426.966	2889.870	-41.930
3700	1005.443	2481.945	1668.346	3010.317	425.450	2958.354	-41.764
3800	1006.714	2508.776	1690.111	3110.925	423.587	3026.823	-41.606
3900	1007.893	2534.941	1711.440	3211.656	421.416	3095.298	-41.456
4000	1008.989	2560.473	1732.347	3312.501	418.921	3163.966	-41.316
4100	1010.010	2585.400	1752.851	3413.452	416.067	3232.628	-41.183
4200	1010.962	2609.750	1772.964	3514.501	412.882	3301.355	-41.058
4300	1011.852	2633.549	1792.702	3615.642	409.351	3370.076	-40.937
4400	1012.684	2656.821	1812.078	3716.869	405.485	3438.972	-40.825
4500	1013.464	2679.588	1831.104	3818.177	401.295	3508.015	-40.719
4600	1014.195	2701.871	1849.792	3919.560	396.732	3577.160	-40.619
4700	1014.882	2723.690	1868.155	4021.015	391.810	3646.299	-40.523
4800	1015.528	2745.063	1886.202	4122.536	386.575	3715.648	-40.434
4900	1016.137	2766.009	1903.944	4224.119	380.955	3784.980	-40.348
5000	1016.710	2786.543	1921.391	4325.762	375.039	3854.612	-40.268

3.303. Hexaphene



Other names: Benzo[*b*]pentaphene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 222-78-6

Point Group: C_s

Length: 18.08 Å

Width: 9.844 Å

Breadth: 3.888 Å

L/B Ratio: 1.837

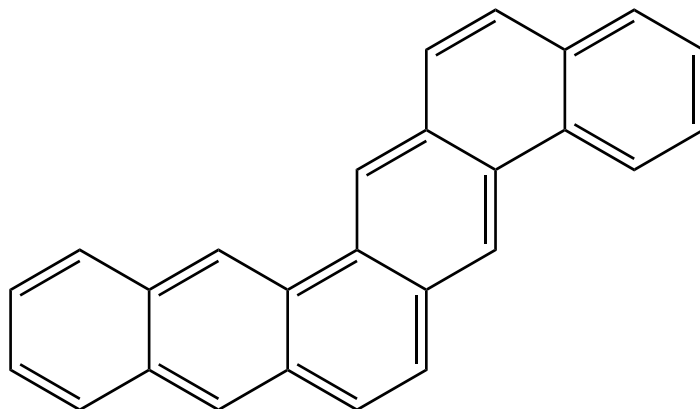
Cartesian coordinates:

C	6.4019	-1.9528	0.0000	C	-0.8609	3.0410	0.0000	H	6.4208	1.4709	0.0000
C	6.9010	-0.6159	0.0000	C	-2.1900	2.8376	0.0000	H	4.6716	-3.2144	0.0000
C	6.0469	0.4407	0.0000	C	-1.8757	0.3741	0.0000	H	4.1198	2.3312	0.0000
C	5.0643	-2.1912	0.0000	C	-2.7502	1.5007	0.0000	H	2.3697	-2.3561	0.0000
C	4.1290	-1.1028	0.0000	C	-4.1191	1.3154	0.0000	H	1.8198	3.1870	0.0000
C	4.6272	0.2316	0.0000	C	-2.4090	-0.9004	0.0000	H	0.0612	-1.4969	0.0000
C	3.7374	1.3030	0.0000	C	-3.8064	-1.1034	0.0000	H	-0.4449	4.0554	0.0000
C	2.7547	-1.3290	0.0000	C	-4.6696	0.0145	0.0000	H	-2.8907	3.6809	0.0000
C	1.8565	-0.2527	0.0000	C	-6.0787	-0.1951	0.0000	H	-4.7946	2.1800	0.0000
C	2.3534	1.0790	0.0000	C	-6.5868	-1.4632	0.0000	H	-1.7320	-1.7700	0.0000
C	1.4285	2.1619	0.0000	C	-5.7202	-2.5851	0.0000	H	-6.7415	0.6775	0.0000
C	0.4490	-0.4652	0.0000	C	-4.3649	-2.4139	0.0000	H	-7.6689	-1.6300	0.0000
C	-0.4308	0.5893	0.0000	H	7.1194	-2.7798	0.0000	H	-6.1550	-3.5900	0.0000
C	0.0746	1.9334	0.0000	H	7.9849	-0.4615	0.0000	H	-3.6880	-3.2756	0.0000

Table 3.303: Table of thermodynamic data as a function of temperature for Hexaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-50.230	442.590	442.590	∞
100	110.895	360.595	792.438	-43.184	468.916	515.913	-269.480
200	215.941	467.855	603.407	-27.110	454.961	568.476	-148.468
250	277.239	522.576	581.744	-14.792	448.416	597.613	-124.862
298.15	337.032	576.532	576.532	0.000	442.590	626.891	-109.826
300	339.302	578.624	576.538	0.626	442.375	628.033	-109.348
350	398.966	635.454	580.890	19.097	437.009	659.413	-98.410
400	454.287	692.395	591.272	40.449	432.353	691.502	-90.299
450	504.408	748.848	605.651	64.439	428.327	724.141	-84.054
500	549.232	804.358	622.755	90.801	424.845	757.220	-79.105
600	624.498	911.418	662.025	149.636	419.220	824.254	-71.756
700	684.176	1012.339	704.937	215.182	415.164	892.107	-66.568
800	732.183	1106.944	749.339	286.084	412.495	960.428	-62.708
900	771.420	1195.523	794.048	361.327	411.037	1029.005	-59.721
1000	803.918	1278.534	838.390	440.144	410.623	1097.699	-57.337
1100	831.115	1356.469	881.983	521.935	411.058	1166.401	-55.387
1200	854.064	1429.797	924.609	606.225	412.199	1235.014	-53.758
1300	873.561	1498.949	966.155	692.632	413.864	1303.521	-52.375
1400	890.226	1564.312	1006.567	780.843	415.923	1371.887	-51.185
1500	904.549	1626.232	1045.833	870.600	418.292	1440.097	-50.148
1600	916.924	1685.015	1083.960	961.688	420.842	1508.133	-49.234
1700	927.668	1740.933	1120.974	1053.930	423.500	1575.982	-48.423
1800	937.040	1794.229	1156.909	1147.176	426.192	1643.736	-47.699
1900	945.253	1845.117	1191.801	1241.299	428.885	1711.289	-47.046
2000	952.482	1893.789	1225.692	1336.194	431.526	1778.727	-46.455
2100	958.870	1940.419	1258.625	1431.768	434.038	1846.021	-45.916
2200	964.539	1985.159	1290.639	1527.944	436.420	1913.203	-45.424
2300	969.587	2028.148	1321.776	1624.655	438.665	1980.277	-44.973
2400	974.101	2069.510	1352.075	1721.844	440.705	2047.212	-44.555
2500	978.149	2109.359	1381.575	1819.460	442.551	2114.175	-44.172
2600	981.792	2147.794	1410.310	1917.460	444.168	2180.956	-43.815
2700	985.081	2184.910	1438.315	2015.806	445.558	2247.748	-43.484
2800	988.059	2220.790	1465.624	2114.466	446.697	2314.516	-43.177
2900	990.763	2255.510	1492.266	2213.409	447.557	2381.195	-42.889
3000	993.225	2289.141	1518.271	2312.610	448.178	2447.874	-42.620
3100	995.472	2321.746	1543.666	2412.047	448.486	2514.464	-42.368
3200	997.528	2353.384	1568.478	2511.698	448.522	2581.119	-42.132
3300	999.414	2384.108	1592.731	2611.547	448.266	2647.814	-41.911
3400	1001.148	2413.970	1616.448	2711.576	447.694	2714.440	-41.701
3500	1002.745	2443.014	1639.651	2811.772	446.807	2781.069	-41.504
3600	1004.219	2471.283	1662.361	2912.121	445.629	2847.810	-41.320
3700	1005.583	2498.817	1684.597	3012.612	444.128	2914.608	-41.146
3800	1006.846	2525.651	1706.379	3113.234	442.278	2981.389	-40.981
3900	1008.019	2551.819	1727.723	3213.978	440.120	3048.177	-40.825
4000	1009.109	2577.354	1748.645	3314.835	437.637	3115.156	-40.679
4100	1010.125	2602.284	1769.163	3415.797	434.795	3182.130	-40.540
4200	1011.072	2626.637	1789.290	3516.858	431.621	3249.169	-40.408
4300	1011.957	2650.439	1809.041	3618.010	428.101	3316.201	-40.283
4400	1012.785	2673.713	1828.429	3719.247	424.245	3383.408	-40.165
4500	1013.560	2696.482	1847.467	3820.565	420.065	3450.761	-40.055
4600	1014.288	2718.767	1866.167	3921.957	415.511	3518.217	-39.950
4700	1014.971	2740.588	1884.541	4023.421	410.599	3585.666	-39.849
4800	1015.614	2761.963	1902.598	4124.950	405.372	3653.325	-39.755
4900	1016.219	2782.911	1920.351	4226.542	399.760	3720.967	-39.665
5000	1016.789	2803.447	1937.808	4328.193	393.853	3788.909	-39.582

3.304. Benzo[*c*]pentaphene



Other names: Anthra[1,2-*b*]phenanthrene
2',3'-Phenanthra-1,2-anthracene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 222-54-8
Point Group: C_s

Length: 18.04 Å
Width: 9.166 Å
Breadth: 3.884 Å
L/B Ratio: 1.968

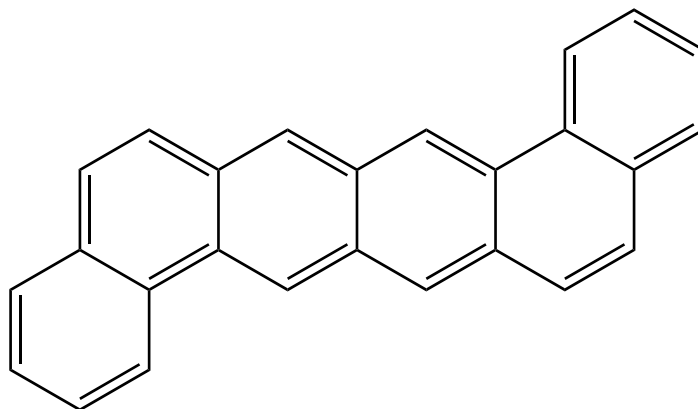
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C	6.0243	0.4736	0.0000	C	-1.7505	-1.0415	0.0000	H	4.3250	2.5717	0.0000
C	4.7478	-2.0236	0.0000	C	-2.4845	0.1650	0.0000	H	2.0405	-1.8746	0.0000
C	3.9553	-0.8376	0.0000	C	-3.8002	-2.3450	0.0000	H	2.1716	3.6957	0.0000
C	4.5987	0.4217	0.0000	C	-2.4486	-2.3004	0.0000	H	-0.3049	3.6022	0.0000
C	3.8215	1.5970	0.0000	C	-4.5793	-1.1351	0.0000	H	-2.3797	2.3195	0.0000
C	2.5481	-0.8964	0.0000	C	-3.9327	0.1129	0.0000	H	0.2283	-1.9395	0.0000
C	1.7875	0.2606	0.0000	C	-4.7099	1.2889	0.0000	H	-4.3340	-3.3024	0.0000
C	2.4385	1.5282	0.0000	C	-6.0856	1.2194	0.0000	H	-1.8528	-3.2204	0.0000
C	1.6422	2.7357	0.0000	C	-6.7289	-0.0277	0.0000	H	-4.1899	2.2593	0.0000
C	0.2958	2.6852	0.0000	C	-5.9881	-1.1895	0.0000	H	-6.6839	2.1363	0.0000
C	0.3316	0.2113	0.0000	H	6.7234	-2.8491	0.0000	H	-7.8230	-0.0705	0.0000
C	-0.4052	1.4209	0.0000	H	7.8505	-0.6442	0.0000	H	-6.4863	-2.1656	0.0000

Table 3.304: Table of thermodynamic data as a function of temperature for Benzo[*c*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.708	417.629	417.629	∞
100	109.720	354.152	782.449	-42.830	444.309	491.951	-256.964
200	214.086	460.384	594.925	-26.908	430.203	545.212	-142.392
250	275.150	514.663	573.419	-14.689	423.558	574.733	-120.082
298.15	334.859	568.242	568.242	0.000	417.629	604.402	-105.886
300	337.127	570.320	568.248	0.622	417.411	605.559	-105.435
350	396.829	626.817	572.574	18.985	411.936	637.363	-95.119
400	452.259	683.479	582.897	40.233	407.176	669.891	-87.477
450	502.524	739.702	597.203	64.124	403.052	702.982	-81.598
500	547.499	795.021	614.228	90.397	399.480	736.523	-76.942
600	623.045	901.791	653.337	149.072	393.696	804.506	-70.037
700	682.949	1002.506	696.099	214.485	389.506	873.332	-65.168
800	731.133	1096.958	740.367	285.273	386.724	942.645	-61.547
900	770.510	1185.422	784.957	360.419	385.168	1012.227	-58.747
1000	803.120	1268.343	829.193	439.150	384.669	1081.936	-56.513
1100	830.408	1346.206	872.692	520.866	385.029	1151.661	-54.687
1200	853.433	1419.476	915.235	605.090	386.103	1221.303	-53.161
1300	872.995	1488.581	956.706	691.437	387.708	1290.844	-51.866
1400	889.716	1553.904	997.051	779.594	389.713	1360.249	-50.750
1500	904.088	1615.791	1036.256	869.302	392.033	1429.501	-49.779
1600	916.504	1674.545	1074.328	960.347	394.540	1498.583	-48.923
1700	927.285	1730.439	1111.293	1052.549	397.158	1567.480	-48.162
1800	936.690	1783.713	1147.181	1145.758	399.813	1636.285	-47.483
1900	944.932	1834.583	1182.032	1239.848	402.473	1704.891	-46.870
2000	952.186	1883.240	1215.884	1334.711	405.083	1773.382	-46.315
2100	958.597	1929.856	1248.781	1430.257	407.566	1841.732	-45.810
2200	964.286	1974.584	1280.762	1526.407	409.922	1909.971	-45.348
2300	969.353	2017.562	1311.869	1623.093	412.143	1978.103	-44.923
2400	973.883	2058.914	1342.140	1720.259	414.161	2046.097	-44.531
2500	977.946	2098.754	1371.612	1817.854	415.986	2114.120	-44.171
2600	981.602	2137.182	1400.323	1915.835	417.582	2181.962	-43.835
2700	984.903	2174.291	1428.305	2014.163	418.954	2249.815	-43.524
2800	987.892	2210.165	1455.592	2112.805	420.076	2317.645	-43.235
2900	990.606	2244.879	1482.213	2211.732	420.920	2385.387	-42.965
3000	993.078	2278.505	1508.199	2310.918	421.526	2453.129	-42.712
3100	995.333	2311.105	1533.576	2410.341	421.820	2520.784	-42.474
3200	997.397	2342.739	1558.370	2509.979	421.842	2588.503	-42.252
3300	999.291	2373.459	1582.607	2609.814	421.574	2656.263	-42.044
3400	1001.031	2403.317	1606.308	2709.832	420.989	2723.954	-41.848
3500	1002.634	2432.358	1629.497	2810.016	420.091	2791.648	-41.662
3600	1004.114	2460.624	1652.193	2910.354	418.902	2859.455	-41.489
3700	1005.483	2488.155	1674.416	3010.835	417.390	2927.319	-41.325
3800	1006.751	2514.987	1696.185	3111.448	415.531	2995.166	-41.171
3900	1007.928	2541.153	1717.516	3212.182	413.364	3063.020	-41.024
4000	1009.023	2566.685	1738.428	3313.031	410.872	3131.067	-40.887
4100	1010.042	2591.613	1758.934	3413.984	408.022	3199.107	-40.756
4200	1010.993	2615.964	1779.051	3515.037	404.840	3267.213	-40.633
4300	1011.881	2639.764	1798.792	3616.181	401.312	3335.313	-40.515
4400	1012.712	2663.036	1818.170	3717.411	397.448	3403.588	-40.405
4500	1013.491	2685.804	1837.199	3818.722	393.261	3472.009	-40.301
4600	1014.221	2708.087	1855.890	3920.108	388.701	3540.532	-40.203
4700	1014.907	2729.907	1874.255	4021.564	383.782	3609.049	-40.109
4800	1015.552	2751.281	1892.304	4123.088	378.549	3677.777	-40.022
4900	1016.160	2772.227	1910.049	4224.674	372.931	3746.487	-39.937
5000	1016.732	2792.762	1927.498	4326.319	367.018	3815.497	-39.859

3.305. Dibenzo[*a,j*]naphthacene



Other names: Dibenzo[*a,j*]tetracene
1,2,7,8-Dibenzotetracene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 227-04-3
Point Group: C_{2h}

Length: 17.79 Å
Width: 8.986 Å
Breadth: 3.885 Å
L/B Ratio: 1.980

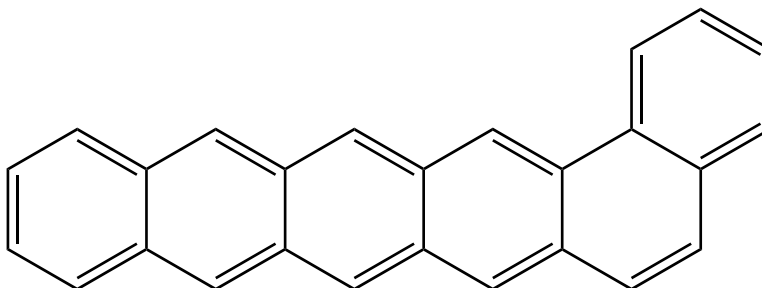
Cartesian coordinates:

C	6.2723	-0.4264	0.0000	C	-0.7871	1.6927	0.0000	H	6.1051	2.9680	0.0000
C	6.6969	0.8879	0.0000	C	-1.5779	-0.9962	0.0000	H	3.6626	2.4544	0.0000
C	5.7611	1.9286	0.0000	C	-2.5360	-0.0016	0.0000	H	2.7995	-3.4476	0.0000
C	4.4097	1.6458	0.0000	C	-2.1299	1.3691	0.0000	H	5.2149	-2.8886	0.0000
C	4.8991	-0.7283	0.0000	C	-3.1384	2.4051	0.0000	H	1.8955	2.0515	0.0000
C	3.9573	0.3145	0.0000	C	-4.4520	2.1015	0.0000	H	0.4718	-2.7436	0.0000
C	3.1384	-2.4050	0.0000	C	-3.9573	-0.3145	0.0000	H	-0.4718	2.7435	0.0000
C	4.4520	-2.1015	0.0000	C	-4.8991	0.7283	0.0000	H	-1.8955	-2.0515	0.0000
C	2.1299	-1.3691	0.0000	C	-6.2723	0.4265	0.0000	H	-2.7995	3.4476	0.0000
C	2.5360	0.0016	0.0000	C	-6.6970	-0.8879	0.0000	H	-5.2149	2.8887	0.0000
C	1.5779	0.9962	0.0000	C	-5.7612	-1.9286	0.0000	H	-7.0026	1.2437	0.0000
C	0.7871	-1.6928	0.0000	C	-4.4097	-1.6458	0.0000	H	-7.7668	-1.1207	0.0000
C	-0.2000	-0.6801	0.0000	H	7.0026	-1.2436	0.0000	H	-6.1052	-2.9680	0.0000
C	0.2000	0.6801	0.0000	H	7.7667	1.1208	0.0000	H	-3.6627	-2.4545	0.0000

Table 3.305: Table of thermodynamic data as a function of temperature for Dibenzo[*a,j*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-50.063	425.101	425.101	∞
100	110.823	352.390	782.817	-43.043	451.568	499.386	-260.847
200	215.127	459.301	594.418	-27.023	437.560	552.785	-144.370
250	276.335	513.828	572.822	-14.749	430.971	582.355	-121.674
298.15	336.135	567.625	567.625	0.000	425.101	612.058	-107.228
300	338.406	569.711	567.631	0.624	424.885	613.216	-106.768
350	398.141	626.408	571.972	19.052	419.476	645.045	-96.266
400	453.558	683.244	582.331	40.365	414.781	677.589	-88.482
450	503.776	739.618	596.682	64.321	410.720	710.689	-82.493
500	548.685	795.066	613.757	90.654	407.209	744.231	-77.748
600	624.078	902.038	652.970	149.441	401.536	812.198	-70.707
700	683.832	1002.901	695.831	214.949	397.442	880.992	-65.739
800	731.882	1097.463	740.189	285.819	394.742	950.260	-62.044
900	771.147	1186.008	784.859	361.034	393.255	1019.786	-59.186
1000	803.664	1268.991	829.168	439.824	392.815	1089.434	-56.905
1100	830.877	1346.903	872.730	521.590	393.225	1159.091	-55.040
1200	853.839	1420.210	915.329	605.858	394.343	1228.662	-53.481
1300	873.350	1489.345	956.850	692.243	395.986	1298.128	-52.158
1400	890.027	1554.694	997.241	780.434	398.025	1367.455	-51.019
1500	904.363	1616.600	1036.486	870.171	400.374	1436.628	-50.027
1600	916.749	1675.371	1074.596	961.241	402.906	1505.627	-49.153
1700	927.504	1731.279	1111.593	1053.466	405.547	1574.441	-48.376
1800	936.887	1784.566	1147.512	1146.696	408.223	1643.161	-47.682
1900	945.110	1835.446	1182.390	1240.805	410.902	1711.681	-47.056
2000	952.348	1884.111	1216.268	1335.686	413.529	1780.086	-46.490
2100	958.745	1930.734	1249.188	1431.247	416.028	1848.349	-45.974
2200	964.421	1975.469	1281.191	1527.410	418.398	1916.499	-45.503
2300	969.477	2018.453	1312.318	1624.110	420.631	1984.542	-45.069
2400	973.997	2059.811	1342.607	1721.288	422.661	2052.447	-44.669
2500	978.051	2099.655	1372.097	1818.894	424.497	2120.380	-44.302
2600	981.700	2138.087	1400.824	1916.885	426.104	2188.132	-43.959
2700	984.994	2175.199	1428.821	2015.222	427.485	2255.895	-43.642
2800	987.977	2211.076	1456.121	2113.873	428.616	2323.634	-43.347
2900	990.686	2245.794	1482.756	2212.809	429.468	2391.284	-43.071
3000	993.152	2279.422	1508.754	2312.002	430.081	2458.935	-42.813
3100	995.403	2312.024	1534.143	2411.432	430.383	2526.497	-42.570
3200	997.463	2343.660	1558.948	2511.076	430.412	2594.124	-42.344
3300	999.352	2374.383	1583.195	2610.919	430.150	2661.792	-42.132
3400	1001.089	2404.242	1606.907	2710.942	429.571	2729.391	-41.931
3500	1002.689	2433.285	1630.104	2811.132	428.679	2796.993	-41.742
3600	1004.166	2461.553	1652.809	2911.475	427.495	2864.707	-41.565
3700	1005.532	2489.085	1675.041	3011.961	425.988	2932.477	-41.398
3800	1006.798	2515.917	1696.818	3112.579	424.134	3000.232	-41.240
3900	1007.972	2542.085	1718.157	3213.318	421.971	3067.993	-41.090
4000	1009.065	2567.618	1739.076	3314.170	419.483	3135.946	-40.950
4100	1010.082	2592.547	1759.589	3415.128	416.637	3203.893	-40.817
4200	1011.031	2616.899	1779.713	3516.184	413.460	3271.906	-40.691
4300	1011.918	2640.700	1799.460	3617.332	409.936	3339.912	-40.571
4400	1012.747	2663.973	1818.845	3718.566	406.075	3408.093	-40.458
4500	1013.524	2686.741	1837.879	3819.880	401.891	3476.420	-40.352
4600	1014.253	2709.026	1856.576	3921.269	397.335	3544.850	-40.252
4700	1014.938	2730.846	1874.946	4022.729	392.418	3613.274	-40.156
4800	1015.582	2752.220	1893.000	4124.256	387.189	3681.907	-40.066
4900	1016.188	2773.167	1910.750	4225.844	381.574	3750.523	-39.980
5000	1016.760	2793.703	1928.204	4327.492	375.663	3819.439	-39.901

3.306. Benzo[*a*]pentacene



Formula: $C_{26}H_{16}$
Mass: 328.405 g/mol
CAS Number: 239-98-5
Point Group: C_s

Length: 18.37 Å
Width: 9.124 Å
Breadth: 3.885 Å
L/B Ratio: 2.013

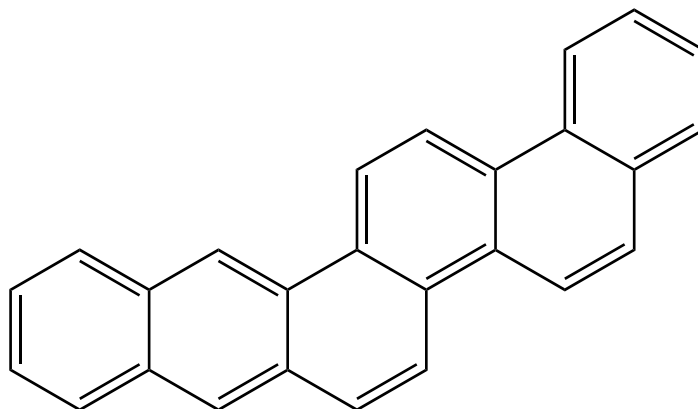
Cartesian coordinates:

C	-6.9823	1.2037	0.0000	C	1.2244	-1.9777	0.0000	H	-6.2223	-2.1379	0.0000
C	-7.1630	-0.2171	0.0000	C	1.5777	0.8080	0.0000	H	-5.5906	2.8279	0.0000
C	-6.0942	-1.0495	0.0000	C	2.6720	-0.0173	0.0000	H	-3.7862	-2.4480	0.0000
C	-5.7391	1.7420	0.0000	C	2.4877	-1.4457	0.0000	H	-3.1545	2.5182	0.0000
C	-4.5717	0.8976	0.0000	C	3.6538	-2.3053	0.0000	H	-1.3551	-2.7567	0.0000
C	-4.7526	-0.5242	0.0000	C	4.9000	-1.7961	0.0000	H	-0.7232	2.2081	0.0000
C	-3.6529	-1.3591	0.0000	C	4.0300	0.5144	0.0000	H	1.0779	-3.0651	0.0000
C	-3.2980	1.4306	0.0000	C	5.1244	-0.3668	0.0000	H	1.7206	1.9009	0.0000
C	-2.1602	0.5871	0.0000	C	6.4312	0.1463	0.0000	H	3.4863	-3.3888	0.0000
C	-2.3401	-0.8273	0.0000	C	6.6443	1.5129	0.0000	H	5.7794	-2.4505	0.0000
C	-1.2146	-1.6686	0.0000	C	5.5578	2.3919	0.0000	H	7.2817	-0.5449	0.0000
C	-0.8598	1.1197	0.0000	C	4.2662	1.8985	0.0000	H	7.6646	1.9100	0.0000
C	0.2508	0.2815	0.0000	H	-7.8722	1.8416	0.0000	H	5.7322	3.4728	0.0000
C	0.0708	-1.1356	0.0000	H	-8.1843	-0.6118	0.0000	H	3.4017	2.5802	0.0000

Table 3.306: Table of thermodynamic data as a function of temperature for Benzo[*a*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-50.267	461.159	461.159	∞
100	111.064	359.103	791.481	-43.238	487.431	534.577	-279.229
200	216.172	466.456	602.207	-27.150	473.490	587.285	-153.380
250	277.650	521.247	580.511	-14.816	466.961	616.490	-128.806
298.15	337.605	575.290	575.290	0.000	461.159	645.830	-113.144
300	339.880	577.385	575.296	0.627	460.945	646.974	-112.646
350	399.670	634.315	579.656	19.131	455.611	678.413	-101.246
400	455.071	691.355	590.055	40.520	450.993	710.557	-92.787
450	505.231	747.904	604.460	64.550	447.007	743.246	-86.272
500	550.063	803.501	621.593	90.954	443.567	776.370	-81.105
600	625.288	910.710	660.926	149.870	438.023	843.481	-73.430
700	684.887	1011.747	703.903	215.491	434.042	911.399	-68.008
800	732.809	1106.441	748.367	286.460	431.440	979.775	-63.971
900	771.966	1195.089	793.131	361.762	430.041	1048.399	-60.846
1000	804.393	1278.154	837.525	440.629	429.678	1117.134	-58.352
1100	831.530	1356.131	881.163	522.465	430.157	1185.871	-56.311
1200	854.427	1429.493	923.831	606.794	431.337	1254.516	-54.607
1300	873.880	1498.673	965.414	693.235	433.036	1323.052	-53.160
1400	890.508	1564.058	1005.861	781.476	435.125	1391.445	-51.914
1500	904.800	1625.997	1045.157	871.259	437.520	1459.679	-50.829
1600	917.148	1684.795	1083.313	962.372	440.094	1527.738	-49.874
1700	927.869	1740.726	1120.352	1054.635	442.773	1595.608	-49.026
1800	937.222	1794.032	1156.310	1147.900	445.484	1663.382	-48.269
1900	945.418	1844.929	1191.224	1242.041	448.195	1730.955	-47.586
2000	952.632	1893.610	1225.135	1336.951	450.851	1798.411	-46.969
2100	959.007	1940.247	1258.085	1432.539	453.378	1865.723	-46.406
2200	964.664	1984.993	1290.116	1528.728	455.773	1932.921	-45.892
2300	969.703	2027.987	1321.269	1625.451	458.030	2000.011	-45.421
2400	974.207	2069.354	1351.583	1722.651	460.082	2066.962	-44.985
2500	978.247	2109.207	1381.096	1820.277	461.938	2133.941	-44.585
2600	981.883	2147.646	1409.844	1918.287	463.564	2200.737	-44.212
2700	985.166	2184.766	1437.861	2016.642	464.963	2267.543	-43.867
2800	988.138	2220.648	1465.181	2115.310	466.111	2334.325	-43.546
2900	990.837	2255.371	1491.833	2214.261	466.977	2401.018	-43.246
3000	993.294	2289.004	1517.848	2313.469	467.606	2467.711	-42.966
3100	995.537	2321.611	1543.252	2412.912	467.921	2534.315	-42.702
3200	997.589	2353.251	1568.073	2512.570	467.963	2600.983	-42.456
3300	999.472	2383.978	1592.334	2612.425	467.713	2667.691	-42.225
3400	1001.202	2413.841	1616.059	2712.460	467.146	2734.330	-42.007
3500	1002.797	2442.887	1639.270	2812.661	466.265	2800.972	-41.801
3600	1004.268	2471.157	1661.987	2913.015	465.091	2867.726	-41.609
3700	1005.629	2498.692	1684.230	3013.511	463.595	2934.536	-41.427
3800	1006.890	2525.527	1706.018	3114.137	461.750	3001.330	-41.255
3900	1008.060	2551.697	1727.368	3214.886	459.596	3068.130	-41.092
4000	1009.149	2577.233	1748.296	3315.747	457.117	3135.121	-40.940
4100	1010.162	2602.164	1768.820	3416.713	454.279	3202.107	-40.795
4200	1011.108	2626.518	1788.952	3517.777	451.109	3269.158	-40.657
4300	1011.991	2650.320	1808.708	3618.932	447.593	3336.202	-40.526
4400	1012.817	2673.595	1828.101	3720.173	443.740	3403.421	-40.403
4500	1013.592	2696.365	1847.144	3821.494	439.563	3470.786	-40.287
4600	1014.318	2718.651	1865.848	3922.890	435.013	3538.253	-40.177
4700	1015.000	2740.472	1884.226	4024.356	430.103	3605.714	-40.072
4800	1015.641	2761.848	1902.288	4125.888	424.879	3673.385	-39.974
4900	1016.245	2782.796	1920.044	4227.483	419.270	3741.038	-39.879
5000	1016.814	2803.333	1937.505	4329.136	413.365	3808.991	-39.791

3.307. Benzo[*b*]picene



Other names: 2,3-Benzopicene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 217-42-5

Point Group: C_s

Length: 18.08 Å

Width: 8.912 Å

Breadth: 3.883 Å

L/B Ratio: 2.028

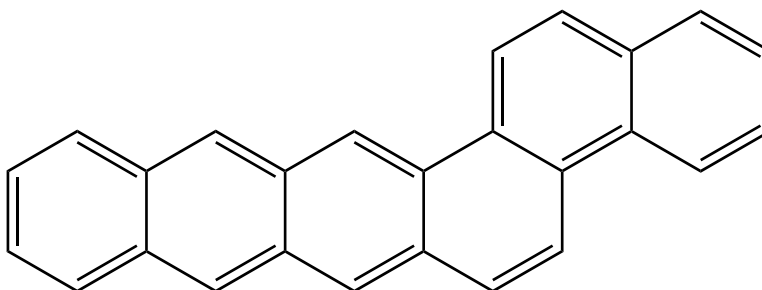
Cartesian coordinates:

C	6.2861	-1.8035	0.0000	C	-1.5793	-1.5685	0.0000	H	6.4209	1.6147	0.0000
C	6.8302	-0.4901	0.0000	C	-0.2226	-1.4080	0.0000	H	4.5086	-3.0026	0.0000
C	6.0105	0.5987	0.0000	C	-2.4435	-0.4436	0.0000	H	4.1468	2.5538	0.0000
C	4.9367	-1.9938	0.0000	C	-1.8942	0.8460	0.0000	H	2.2304	-2.0632	0.0000
C	4.0487	-0.8740	0.0000	C	-2.7730	1.9801	0.0000	H	1.9001	3.4964	0.0000
C	4.5909	0.4346	0.0000	C	-4.1199	1.8279	0.0000	H	-0.5616	3.1897	0.0000
C	3.7259	1.5406	0.0000	C	-3.8778	-0.6134	0.0000	H	-2.0313	-2.5724	0.0000
C	2.6557	-1.0467	0.0000	C	-4.7082	0.5212	0.0000	H	0.4495	-2.2799	0.0000
C	1.7994	0.0478	0.0000	C	-6.1123	0.3616	0.0000	H	-2.3181	2.9823	0.0000
C	2.3483	1.3607	0.0000	C	-6.6673	-0.8962	0.0000	H	-4.7852	2.6990	0.0000
C	1.4583	2.4932	0.0000	C	-5.8402	-2.0337	0.0000	H	-6.7504	1.2526	0.0000
C	0.1182	2.3241	0.0000	C	-4.4726	-1.8957	0.0000	H	-7.7550	-1.0219	0.0000
C	0.3564	-0.1133	0.0000	H	6.9711	-2.6578	0.0000	H	-6.2949	-3.0297	0.0000
C	-0.4737	1.0109	0.0000	H	7.9185	-0.3704	0.0000	H	-3.8145	-2.7779	0.0000

Table 3.307: Table of thermodynamic data as a function of temperature for Benzo[*b*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-50.114	423.861	423.861	∞
100	111.363	361.188	791.332	-43.014	450.357	497.295	-259.755
200	214.987	468.297	603.150	-26.971	436.373	549.799	-143.590
250	275.779	522.748	581.601	-14.713	429.766	578.920	-120.956
298.15	335.234	576.416	576.416	0.000	423.861	608.197	-106.551
300	337.493	578.497	576.422	0.622	423.644	609.339	-106.093
350	396.970	635.032	580.751	18.998	418.181	640.732	-95.622
400	452.229	691.701	591.080	40.248	413.424	672.850	-87.863
450	502.369	747.913	605.390	64.135	409.295	705.530	-81.894
500	547.256	803.211	622.416	90.397	405.713	738.661	-77.166
600	622.693	909.926	661.521	149.043	399.898	805.827	-70.152
700	682.536	1010.581	704.272	214.417	395.670	873.843	-65.206
800	730.684	1104.976	748.524	285.162	392.845	942.352	-61.528
900	770.043	1193.386	793.095	360.262	391.243	1011.134	-58.683
1000	802.647	1276.258	837.312	438.946	390.697	1080.049	-56.415
1100	829.941	1354.076	880.790	520.614	391.010	1148.985	-54.560
1200	852.978	1427.305	923.312	604.792	392.037	1217.842	-53.010
1300	872.557	1496.374	964.762	691.095	393.598	1286.602	-51.695
1400	889.298	1561.666	1005.088	779.209	395.560	1355.230	-50.563
1500	903.690	1623.524	1044.273	868.876	397.840	1423.707	-49.577
1600	916.129	1682.254	1082.327	959.882	400.307	1492.017	-48.708
1700	926.932	1738.125	1119.274	1052.048	402.889	1560.145	-47.936
1800	936.358	1791.380	1155.145	1145.223	405.510	1628.181	-47.248
1900	944.620	1842.233	1189.980	1239.280	408.138	1696.021	-46.626
2000	951.893	1890.874	1223.817	1334.114	410.717	1763.749	-46.063
2100	958.322	1937.476	1256.699	1429.631	413.172	1831.336	-45.551
2200	964.028	1982.191	1288.667	1525.754	415.501	1898.813	-45.083
2300	969.110	2025.158	1319.760	1622.416	417.697	1966.185	-44.653
2400	973.654	2066.501	1350.018	1719.558	419.691	2033.420	-44.255
2500	977.731	2106.332	1379.479	1817.131	421.494	2100.685	-43.891
2600	981.400	2144.752	1408.178	1915.091	423.070	2167.770	-43.550
2700	984.713	2181.853	1436.150	2013.399	424.422	2234.866	-43.235
2800	987.712	2217.720	1463.426	2112.023	425.526	2301.941	-42.942
2900	990.436	2252.428	1490.038	2210.932	426.352	2368.927	-42.668
3000	992.917	2286.048	1516.014	2310.102	426.941	2435.915	-42.412
3100	995.181	2318.643	1541.382	2409.509	427.220	2502.815	-42.171
3200	997.253	2350.272	1566.168	2509.132	427.227	2569.780	-41.946
3300	999.153	2380.989	1590.397	2608.953	426.945	2636.787	-41.736
3400	1000.901	2410.843	1614.091	2708.957	426.347	2703.725	-41.537
3500	1002.510	2439.880	1637.272	2809.129	425.436	2770.668	-41.349
3600	1003.996	2468.143	1659.961	2909.455	424.234	2837.723	-41.173
3700	1005.370	2495.670	1682.177	3009.924	422.712	2904.834	-41.008
3800	1006.644	2522.499	1703.939	3110.526	420.841	2971.931	-40.851
3900	1007.826	2548.662	1725.265	3211.250	418.663	3039.034	-40.702
4000	1008.925	2574.192	1746.170	3312.088	416.162	3106.329	-40.564
4100	1009.948	2599.118	1766.671	3413.033	413.302	3173.619	-40.432
4200	1010.903	2623.467	1786.782	3514.076	410.111	3240.975	-40.307
4300	1011.795	2647.264	1806.518	3615.211	406.574	3308.325	-40.187
4400	1012.630	2670.535	1825.891	3716.433	402.702	3375.850	-40.076
4500	1013.412	2693.300	1844.915	3817.735	398.507	3443.521	-39.971
4600	1014.145	2715.582	1863.601	3919.114	393.939	3511.294	-39.871
4700	1014.834	2737.400	1881.961	4020.563	389.012	3579.063	-39.776
4800	1015.482	2758.772	1900.006	4122.079	383.772	3647.040	-39.687
4900	1016.092	2779.717	1917.746	4223.658	378.147	3715.002	-39.602
5000	1016.667	2800.251	1935.192	4325.296	372.228	3783.263	-39.523

3.308. Naphtho[2,1-*a*]naphthacene



Other names: Naphtho[2'.1',1.2]tetracene
Naphtho[*b'*,*b*]chrysene

Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 220-82-6
Point Group: C_s

Length: 18.41 Å
Width: 9.011 Å
Breadth: 3.884 Å
L/B Ratio: 2.043

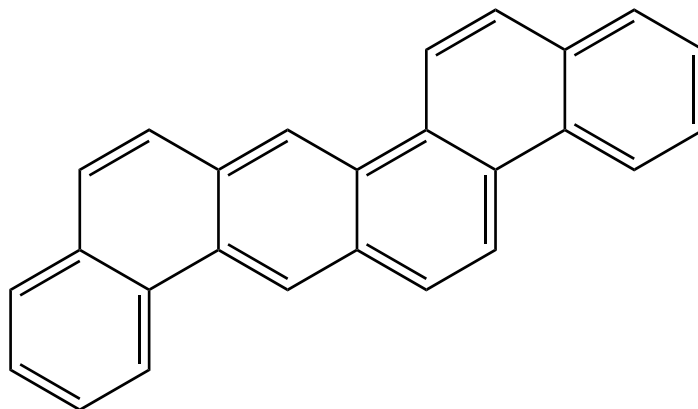
Cartesian coordinates:

C	6.7619	-1.3611	0.0000	C	-1.1893	2.4297	0.0000	H	6.2491	2.0253	0.0000
C	7.0470	0.0393	0.0000	C	-2.4704	2.0058	0.0000	H	5.2511	-2.8771	0.0000
C	6.0403	0.9494	0.0000	C	-1.7755	-0.3425	0.0000	H	3.8420	2.5160	0.0000
C	5.4795	-1.8052	0.0000	C	-2.7966	0.6018	0.0000	H	2.8440	-2.3877	0.0000
C	4.3829	-0.8760	0.0000	C	-3.3937	-2.1510	0.0000	H	1.4356	3.0015	0.0000
C	4.6677	0.5229	0.0000	C	-2.0986	-1.7308	0.0000	H	0.4347	-1.8998	0.0000
C	3.6262	1.4404	0.0000	C	-4.4599	-1.2047	0.0000	H	-0.9483	3.4990	0.0000
C	3.0656	-1.3134	0.0000	C	-4.1672	0.1729	0.0000	H	-3.3082	2.7200	0.0000
C	2.0043	-0.3890	0.0000	C	-5.2424	1.0984	0.0000	H	-3.6375	-3.2195	0.0000
C	2.2881	1.0044	0.0000	C	-6.5419	0.6627	0.0000	H	-1.2684	-2.4539	0.0000
C	1.2128	1.9271	0.0000	C	-6.8302	-0.7183	0.0000	H	-5.0058	2.1733	0.0000
C	0.6549	-0.8201	0.0000	C	-5.8110	-1.6351	0.0000	H	-7.3675	1.3818	0.0000
C	-0.3857	0.0859	0.0000	H	7.6004	-2.0651	0.0000	H	-7.8744	-1.0474	0.0000
C	-0.0951	1.4889	0.0000	H	8.0940	0.3595	0.0000	H	-6.0252	-2.7099	0.0000

Table 3.308: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.748	443.941	443.941	∞
100	109.867	354.134	782.829	-42.870	470.582	518.225	-270.687
200	214.321	460.488	595.137	-26.930	456.493	571.481	-149.252
250	275.384	514.821	573.616	-14.699	449.860	600.996	-125.569
298.15	335.011	568.435	568.435	0.000	443.941	630.656	-110.486
300	337.276	570.515	568.442	0.622	443.723	631.813	-110.006
350	396.857	627.025	572.769	18.990	438.253	663.606	-99.036
400	452.175	683.684	583.094	40.236	433.491	696.124	-90.903
450	502.350	739.891	597.400	64.121	429.360	729.205	-84.642
500	547.260	795.189	614.423	90.383	425.778	762.738	-79.681
600	622.735	901.907	653.523	149.031	419.966	830.706	-72.318
700	682.615	1002.572	696.271	214.411	415.744	899.523	-67.122
800	730.798	1096.980	740.524	285.165	412.928	968.832	-63.257
900	770.184	1185.405	785.096	360.278	411.339	1038.413	-60.267
1000	802.809	1268.292	829.315	438.977	410.808	1108.126	-57.881
1100	830.115	1346.127	872.797	520.663	411.138	1177.857	-55.931
1200	853.159	1419.372	915.323	604.858	412.183	1247.509	-54.302
1300	872.739	1488.455	956.779	691.179	413.762	1317.061	-52.919
1400	889.478	1553.760	997.109	779.312	415.743	1386.480	-51.729
1500	903.866	1615.631	1036.300	868.997	418.040	1455.747	-50.693
1600	916.299	1674.372	1074.359	960.020	420.525	1524.846	-49.780
1700	927.095	1730.253	1111.311	1052.202	423.123	1593.761	-48.969
1800	936.513	1783.517	1147.188	1145.393	425.760	1662.584	-48.246
1900	944.768	1834.378	1182.027	1239.466	428.403	1731.210	-47.593
2000	952.033	1883.027	1215.870	1334.314	430.997	1799.723	-47.003
2100	958.455	1929.635	1248.757	1429.844	433.465	1868.095	-46.465
2200	964.153	1974.357	1280.729	1525.980	435.807	1936.356	-45.974
2300	969.229	2017.329	1311.827	1622.654	438.015	2004.511	-45.523
2400	973.767	2058.677	1342.090	1719.808	440.021	2072.528	-45.106
2500	977.837	2098.512	1371.555	1817.392	441.835	2140.576	-44.724
2600	981.500	2136.936	1400.258	1915.362	443.421	2208.442	-44.367
2700	984.808	2174.041	1428.234	2013.680	444.783	2276.320	-44.037
2800	987.802	2209.911	1455.514	2112.313	445.896	2344.175	-43.730
2900	990.522	2244.623	1482.129	2211.232	446.731	2411.942	-43.443
3000	992.998	2278.245	1508.109	2310.410	447.329	2479.710	-43.175
3100	995.258	2310.843	1533.480	2409.824	447.615	2547.391	-42.922
3200	997.326	2342.474	1558.270	2509.455	447.630	2615.136	-42.687
3300	999.223	2373.193	1582.501	2609.284	447.355	2682.923	-42.466
3400	1000.967	2403.049	1606.198	2709.294	446.763	2750.640	-42.258
3500	1002.573	2432.088	1629.382	2809.472	445.859	2818.362	-42.061
3600	1004.056	2460.353	1652.074	2909.805	444.664	2886.196	-41.877
3700	1005.428	2487.882	1674.293	3010.280	443.147	2954.087	-41.703
3800	1006.698	2514.712	1696.057	3110.887	441.282	3021.962	-41.539
3900	1007.878	2540.877	1717.385	3211.616	439.109	3089.843	-41.383
4000	1008.975	2566.408	1738.293	3312.460	436.613	3157.917	-41.237
4100	1009.996	2591.335	1758.796	3413.409	433.758	3225.986	-41.099
4200	1010.949	2615.685	1778.909	3514.457	430.572	3294.120	-40.968
4300	1011.840	2639.484	1798.647	3615.597	427.040	3362.248	-40.842
4400	1012.672	2662.755	1818.022	3716.823	423.172	3430.550	-40.725
4500	1013.453	2685.521	1837.048	3818.129	418.980	3498.999	-40.614
4600	1014.184	2707.804	1855.736	3919.512	414.417	3567.551	-40.510
4700	1014.872	2729.623	1874.098	4020.965	409.494	3636.097	-40.410
4800	1015.518	2750.996	1892.145	4122.485	404.258	3704.852	-40.316
4900	1016.127	2771.942	1909.887	4224.067	398.636	3773.591	-40.226
5000	1016.701	2792.476	1927.334	4325.709	392.720	3842.630	-40.143

3.309. Naphtho[1,2-*b*]chrysene



Other names: Dibenzo[*c,k*]tetraphene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 220-77-9

Point Group: C_s

Length: 17.99 Å

Width: 8.726 Å

Breadth: 3.884 Å

L/B Ratio: 2.062

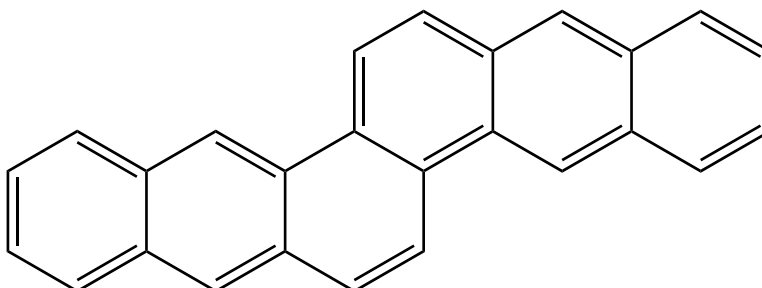
Cartesian coordinates:

C	6.1648	-0.5706	0.0000	C	-0.6988	2.1345	0.0000	H	6.2717	2.8258	0.0000
C	6.6929	0.7036	0.0000	C	-2.0386	1.9332	0.0000	H	3.7946	2.5121	0.0000
C	5.8432	1.8184	0.0000	C	-1.7390	-0.4932	0.0000	H	2.4510	-3.2943	0.0000
C	4.4751	1.6467	0.0000	C	-2.5914	0.6096	0.0000	H	4.9065	-2.9393	0.0000
C	4.7696	-0.7615	0.0000	C	-3.6343	-2.0102	0.0000	H	1.9996	2.2542	0.0000
C	3.9157	0.3546	0.0000	C	-2.2895	-1.8111	0.0000	H	0.1818	-2.3990	0.0000
C	2.8759	-2.2839	0.0000	C	-4.5317	-0.8989	0.0000	H	-0.2807	3.1476	0.0000
C	4.2126	-2.0908	0.0000	C	-4.0167	0.4111	0.0000	H	-2.7423	2.7799	0.0000
C	1.9636	-1.1669	0.0000	C	-4.9224	1.5007	0.0000	H	-4.0528	-3.0231	0.0000
C	2.4779	0.1551	0.0000	C	-6.2773	1.2854	0.0000	H	-1.5892	-2.6605	0.0000
C	1.5930	1.2298	0.0000	C	-6.7887	-0.0279	0.0000	H	-4.5113	2.5217	0.0000
C	0.5871	-1.3742	0.0000	C	-5.9336	-1.1011	0.0000	H	-6.9723	2.1314	0.0000
C	-0.3066	-0.2954	0.0000	H	6.8259	-1.4447	0.0000	H	-7.8727	-0.1814	0.0000
C	0.2084	1.0227	0.0000	H	7.7778	0.8508	0.0000	H	-6.3226	-2.1256	0.0000

Table 3.309: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-50.233	414.274	414.274	∞
100	111.768	362.093	793.134	-43.104	440.679	487.527	-254.653
200	215.423	469.470	604.577	-27.021	426.734	539.926	-141.011
250	276.299	524.027	582.987	-14.740	420.151	568.986	-118.881
298.15	335.837	577.793	577.793	0.000	414.274	598.198	-104.800
300	338.099	579.878	577.800	0.623	414.057	599.338	-104.352
350	397.648	636.512	582.136	19.032	408.627	630.660	-94.119
400	452.953	693.275	592.483	40.317	403.904	662.701	-86.538
450	503.114	749.574	606.817	64.241	399.812	695.300	-80.707
500	548.001	804.951	623.870	90.540	396.268	728.346	-76.088
600	623.402	911.798	663.034	149.259	390.526	795.332	-69.238
700	683.188	1012.559	705.844	214.701	386.366	863.155	-64.408
800	731.277	1107.037	750.153	285.508	383.603	931.461	-60.817
900	770.579	1195.513	794.776	360.664	382.058	1000.034	-58.039
1000	803.133	1278.439	839.040	439.399	381.563	1068.734	-55.824
1100	830.381	1356.301	882.561	521.114	381.922	1137.449	-54.012
1200	853.377	1429.567	925.122	605.334	382.991	1206.082	-52.498
1300	872.920	1498.666	966.609	691.675	384.590	1274.614	-51.214
1400	889.628	1563.984	1006.967	779.823	386.587	1343.011	-50.107
1500	903.992	1625.864	1046.183	869.522	388.898	1411.256	-49.143
1600	916.405	1684.612	1084.264	960.557	391.394	1479.330	-48.294
1700	927.185	1740.500	1121.236	1052.749	394.002	1547.221	-47.539
1800	936.591	1793.769	1157.131	1145.948	396.648	1615.020	-46.866
1900	944.835	1844.633	1191.987	1240.028	399.298	1682.620	-46.258
2000	952.091	1893.285	1225.844	1334.882	401.898	1750.107	-45.707
2100	958.506	1939.896	1258.745	1430.419	404.372	1817.453	-45.206
2200	964.198	1984.620	1290.729	1526.559	406.719	1884.688	-44.747
2300	969.269	2027.594	1321.839	1623.237	408.931	1951.817	-44.326
2400	973.802	2068.943	1352.112	1720.395	410.941	2018.808	-43.937
2500	977.869	2108.780	1381.587	1817.982	412.758	2085.828	-43.580
2600	981.529	2147.205	1410.299	1915.955	414.347	2152.667	-43.247
2700	984.833	2184.311	1438.283	2014.276	415.712	2219.519	-42.938
2800	987.825	2220.182	1465.571	2112.912	416.827	2286.347	-42.651
2900	990.543	2254.895	1492.194	2211.832	417.664	2353.087	-42.383
3000	993.017	2288.518	1518.181	2311.012	418.264	2419.828	-42.132
3100	995.275	2321.116	1543.559	2410.428	418.552	2486.481	-41.896
3200	997.342	2352.748	1568.354	2510.061	418.568	2553.199	-41.676
3300	999.238	2383.467	1592.591	2609.891	418.295	2619.958	-41.470
3400	1000.981	2413.324	1616.293	2709.903	417.705	2686.648	-41.274
3500	1002.586	2442.363	1639.482	2810.083	416.802	2753.342	-41.091
3600	1004.068	2470.628	1662.179	2910.416	415.608	2820.149	-40.918
3700	1005.439	2498.157	1684.403	3010.892	414.092	2887.012	-40.756
3800	1006.709	2524.988	1706.172	3111.501	412.228	2953.859	-40.603
3900	1007.888	2551.153	1727.504	3212.231	410.057	3020.713	-40.457
4000	1008.984	2576.684	1748.416	3313.075	407.561	3087.759	-40.321
4100	1010.005	2601.612	1768.922	3414.025	404.707	3154.800	-40.192
4200	1010.957	2625.962	1789.039	3515.074	401.522	3221.907	-40.069
4300	1011.847	2649.761	1808.780	3616.215	397.990	3289.007	-39.953
4400	1012.680	2673.032	1828.159	3717.442	394.123	3356.282	-39.843
4500	1013.459	2695.799	1847.188	3818.749	389.933	3423.703	-39.740
4600	1014.191	2718.082	1865.879	3920.132	385.369	3491.227	-39.643
4700	1014.878	2739.900	1884.244	4021.586	380.447	3558.745	-39.550
4800	1015.524	2761.274	1902.293	4123.106	375.212	3626.473	-39.463
4900	1016.133	2782.220	1920.038	4224.689	369.591	3694.184	-39.380
5000	1016.706	2802.754	1937.488	4326.331	363.675	3762.195	-39.303

3.310. Dibenzo[*b,k*]chrysene



Other names: Anthraceno[2,1-*a*]anthracene

Formula: C₂₆H₁₆

Mass: 328.405 g/mol

CAS Number: 217-54-9

Point Group: C_{2h}

Length: 18.42 Å

Width: 8.732 Å

Breadth: 3.886 Å

L/B Ratio: 2.109

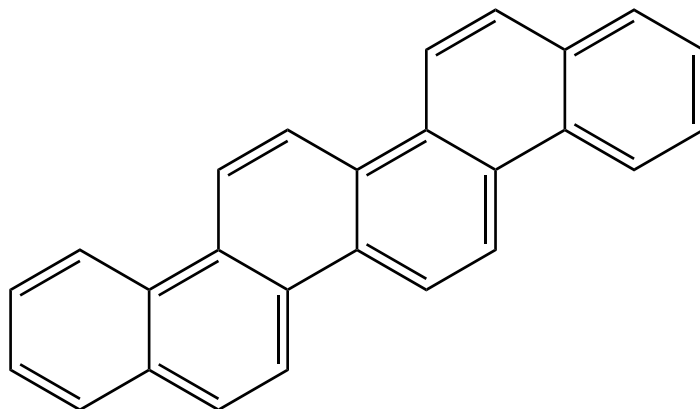
Cartesian coordinates:

C	6.6219	-1.1837	0.0000	C	-1.1583	-2.2634	0.0000	H	6.1963	2.2115	0.0000
C	6.9439	0.2026	0.0000	C	0.1380	-1.8734	0.0000	H	5.0659	-2.6577	0.0000
C	5.9581	1.1418	0.0000	C	-2.2181	-1.2931	0.0000	H	3.7989	2.7647	0.0000
C	5.3231	-1.5925	0.0000	C	-1.8911	0.0915	0.0000	H	2.6667	-2.1043	0.0000
C	4.2616	-0.6331	0.0000	C	-2.9190	1.0318	0.0000	H	1.4274	3.3259	0.0000
C	4.5826	0.7482	0.0000	C	-3.5512	-1.6960	0.0000	H	-0.9545	2.6117	0.0000
C	3.5511	1.6960	0.0000	C	-4.5826	-0.7482	0.0000	H	-1.4274	-3.3260	0.0000
C	2.9191	-1.0318	0.0000	C	-4.2616	0.6332	0.0000	H	0.9544	-2.6119	0.0000
C	1.8911	-0.0916	0.0000	C	-5.3231	1.5926	0.0000	H	-2.6666	2.1043	0.0000
C	2.2180	1.2930	0.0000	C	-6.6219	1.1838	0.0000	H	-3.7989	-2.7647	0.0000
C	1.1583	2.2633	0.0000	C	-6.9439	-0.2025	0.0000	H	-5.0658	2.6578	0.0000
C	-0.1380	1.8733	0.0000	C	-5.9582	-1.1418	0.0000	H	-7.4382	1.9136	0.0000
C	0.4973	-0.4837	0.0000	H	7.4382	-1.9135	0.0000	H	-7.9982	-0.4978	0.0000
C	-0.4973	0.4837	0.0000	H	7.9982	0.4979	0.0000	H	-6.1964	-2.2114	0.0000

Table 3.310: Table of thermodynamic data as a function of temperature for Dibenzo[*b,k*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	–49.572	435.400	435.400	∞
100	109.295	345.775	773.493	–42.772	462.138	510.617	–266.714
200	213.832	451.780	586.191	–26.882	448.000	564.729	–147.489
250	274.895	506.004	564.705	–14.675	441.343	594.683	–124.250
298.15	334.537	559.533	559.533	0.000	435.400	624.769	–109.455
300	336.803	561.610	559.540	0.621	435.181	625.943	–108.984
350	396.407	618.049	563.861	18.966	429.688	658.183	–98.226
400	451.750	674.649	574.173	40.190	424.904	691.151	–90.253
450	501.950	730.807	588.464	64.055	420.753	724.686	–84.118
500	546.886	786.064	605.470	90.297	417.151	758.673	–79.256
600	622.410	892.719	644.536	148.910	411.304	827.557	–72.044
700	682.334	993.337	687.252	214.260	407.052	897.296	–66.956
800	730.555	1087.710	731.475	284.988	404.210	967.530	–63.172
900	769.973	1176.108	776.021	360.078	402.598	1038.039	–60.245
1000	802.625	1258.975	820.217	438.758	402.048	1108.683	–57.910
1100	829.954	1336.793	863.678	520.426	402.360	1179.347	–56.001
1200	853.017	1410.025	906.186	604.606	403.390	1249.932	–54.407
1300	872.613	1479.097	947.625	690.914	404.956	1320.420	–53.054
1400	889.366	1544.394	987.940	779.034	406.924	1390.775	–51.889
1500	903.766	1606.257	1027.118	868.709	409.211	1460.980	–50.875
1600	916.208	1664.991	1065.165	959.722	411.686	1531.015	–49.981
1700	927.013	1720.868	1102.106	1051.896	414.276	1600.869	–49.188
1800	936.439	1774.127	1137.972	1145.079	416.905	1670.631	–48.479
1900	944.700	1824.984	1172.803	1239.145	419.541	1740.197	–47.840
2000	951.971	1873.630	1206.637	1333.986	422.128	1809.649	–47.262
2100	958.398	1920.235	1239.516	1429.511	424.591	1878.960	–46.736
2200	964.101	1964.954	1271.481	1525.642	426.928	1948.161	–46.254
2300	969.181	2007.924	1302.572	1622.311	429.131	2017.257	–45.812
2400	973.722	2049.270	1332.828	1719.460	431.132	2086.215	–45.404
2500	977.796	2089.103	1362.288	1817.039	432.941	2155.203	–45.030
2600	981.462	2127.526	1390.985	1915.005	434.523	2224.010	–44.680
2700	984.772	2164.630	1418.956	2013.320	435.882	2292.829	–44.357
2800	987.769	2200.499	1446.231	2111.949	436.991	2361.626	–44.056
2900	990.490	2235.209	1472.842	2210.864	437.822	2430.334	–43.774
3000	992.968	2268.830	1498.817	2310.039	438.417	2499.044	–43.511
3100	995.230	2301.427	1524.185	2409.451	438.701	2567.666	–43.264
3200	997.300	2333.058	1548.970	2509.079	438.713	2636.353	–43.033
3300	999.198	2363.776	1573.198	2608.905	438.435	2705.081	–42.817
3400	1000.943	2393.631	1596.892	2708.913	437.841	2773.740	–42.612
3500	1002.551	2422.669	1620.072	2809.089	436.935	2842.404	–42.420
3600	1004.035	2450.933	1642.761	2909.419	435.737	2911.180	–42.239
3700	1005.408	2478.462	1664.977	3009.893	434.218	2980.012	–42.069
3800	1006.680	2505.291	1686.739	3110.498	432.352	3048.830	–41.908
3900	1007.860	2531.456	1708.064	3211.225	430.177	3117.653	–41.755
4000	1008.958	2556.986	1728.970	3312.067	427.679	3186.669	–41.613
4100	1009.980	2581.913	1749.470	3413.014	424.822	3255.680	–41.477
4200	1010.934	2606.263	1769.581	3514.061	421.635	3324.756	–41.349
4300	1011.825	2630.061	1789.317	3615.199	418.101	3393.826	–41.226
4400	1012.658	2653.332	1808.690	3716.424	414.232	3463.071	–41.111
4500	1013.439	2676.098	1827.714	3817.729	410.039	3532.463	–41.003
4600	1014.171	2698.380	1846.400	3919.110	405.474	3601.957	–40.901
4700	1014.859	2720.199	1864.760	4020.562	400.550	3671.445	–40.803
4800	1015.506	2741.572	1882.805	4122.080	395.312	3741.143	–40.711
4900	1016.116	2762.517	1900.546	4223.662	389.690	3810.824	–40.623
5000	1016.690	2783.051	1917.991	4325.302	383.772	3880.805	–40.542

3.311. Benzo[*c*]picene



Formula: C₂₆H₁₆
Mass: 328.405 g/mol
CAS Number: 217-37-8
Point Group: C_{2h}

Length: 18.04 Å
Width: 7.960 Å
Breadth: 3.884 Å
L/B Ratio: 2.266

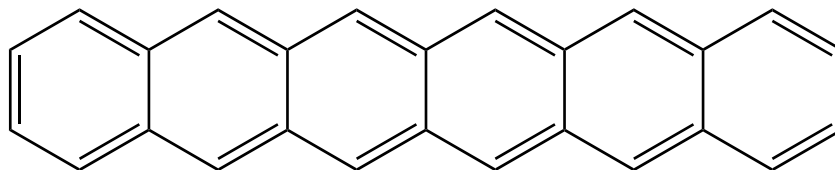
Cartesian coordinates:

C	6.1325	-1.4235	0.0000	C	-0.4967	1.8030	0.0000	H	6.4510	1.9723	0.0000
C	6.7470	-0.1571	0.0000	C	-1.8551	1.7193	0.0000	H	4.2702	-2.5128	0.0000
C	5.9801	0.9827	0.0000	C	-1.7455	-0.7151	0.0000	H	4.2607	3.0498	0.0000
C	4.7631	-1.5286	0.0000	C	-2.5110	0.4546	0.0000	H	1.7802	2.8910	0.0000
C	3.9506	-0.3703	0.0000	C	-3.7605	-2.0745	0.0000	H	-0.0079	-2.7812	0.0000
C	4.5684	0.8932	0.0000	C	-2.4064	-1.9857	0.0000	H	2.4806	-2.6254	0.0000
C	3.7605	2.0745	0.0000	C	-4.5685	-0.8932	0.0000	H	0.0080	2.7811	0.0000
C	2.4063	1.9857	0.0000	C	-3.9506	0.3704	0.0000	H	-2.4804	2.6254	0.0000
C	2.5110	-0.4546	0.0000	C	-4.7631	1.5287	0.0000	H	-4.2607	-3.0498	0.0000
C	1.7456	0.7151	0.0000	C	-6.1325	1.4235	0.0000	H	-1.7802	-2.8910	0.0000
C	0.4968	-1.8030	0.0000	C	-6.7471	0.1571	0.0000	H	-4.2703	2.5129	0.0000
C	1.8552	-1.7193	0.0000	C	-5.9802	-0.9826	0.0000	H	-6.7562	2.3234	0.0000
C	-0.3114	-0.6284	0.0000	H	6.7562	-2.3233	0.0000	H	-7.8399	0.0903	0.0000
C	0.3114	0.6284	0.0000	H	7.8398	-0.0903	0.0000	H	-6.4510	-1.9722	0.0000

Table 3.311: Table of thermodynamic data as a function of temperature for Benzo[*c*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-49.902	413.793	413.793	∞
100	111.092	352.201	780.771	-42.857	440.446	488.282	-255.047
200	214.126	458.913	593.283	-26.874	426.401	541.704	-141.476
250	274.779	513.155	571.809	-14.663	419.747	571.299	-119.364
298.15	334.182	566.641	566.641	0.000	413.793	601.042	-105.298
300	336.441	568.715	566.648	0.620	413.573	602.203	-104.851
350	395.935	625.089	570.964	18.944	408.058	634.089	-94.631
400	451.249	681.623	581.265	40.144	403.250	666.707	-87.061
450	501.461	737.724	595.539	63.983	399.074	699.894	-81.240
500	546.421	792.930	612.527	90.202	395.448	733.537	-76.631
600	621.985	899.504	651.553	148.770	389.557	801.739	-69.796
700	681.922	1000.058	694.232	214.078	385.263	870.803	-64.979
800	730.138	1094.376	738.419	284.765	382.380	940.367	-61.398
900	769.548	1182.724	782.931	359.813	380.726	1010.213	-58.630
1000	802.194	1265.546	827.096	438.450	380.133	1080.197	-56.423
1100	829.523	1343.322	870.527	520.075	380.402	1150.206	-54.618
1200	852.592	1416.517	913.006	604.213	381.390	1220.140	-53.110
1300	872.200	1485.556	954.419	690.479	382.913	1289.980	-51.831
1400	888.967	1550.823	994.709	778.558	384.841	1359.691	-50.730
1500	903.384	1612.659	1033.863	868.194	387.088	1429.254	-49.770
1600	915.845	1671.369	1071.888	959.170	389.527	1498.651	-48.925
1700	926.669	1727.224	1108.808	1051.308	392.081	1567.868	-48.174
1800	936.114	1780.465	1144.655	1144.458	394.677	1636.996	-47.503
1900	944.393	1831.304	1179.466	1238.492	397.281	1705.928	-46.898
2000	951.682	1879.935	1213.283	1333.304	399.838	1774.749	-46.351
2100	958.125	1926.526	1246.145	1428.800	402.273	1843.431	-45.852
2200	963.844	1971.233	1278.095	1524.905	404.583	1912.003	-45.396
2300	968.939	2014.192	1309.171	1621.549	406.761	1980.471	-44.977
2400	973.494	2055.528	1339.414	1718.674	408.739	2048.803	-44.590
2500	977.581	2095.352	1368.860	1816.232	410.526	2117.166	-44.235
2600	981.259	2133.767	1397.545	1914.177	412.087	2185.349	-43.903
2700	984.580	2170.863	1425.503	2012.472	413.426	2253.544	-43.597
2800	987.587	2206.725	1452.767	2111.082	414.517	2321.717	-43.311
2900	990.319	2241.429	1479.367	2209.980	415.330	2389.804	-43.044
3000	992.805	2275.045	1505.332	2309.138	415.909	2457.892	-42.795
3100	995.076	2307.636	1530.690	2408.534	416.176	2525.892	-42.560
3200	997.153	2339.262	1555.466	2508.147	416.173	2593.958	-42.341
3300	999.059	2369.976	1579.685	2607.959	415.881	2662.067	-42.136
3400	1000.811	2399.827	1603.370	2707.953	415.274	2730.106	-41.942
3500	1002.425	2428.862	1626.543	2808.116	414.355	2798.150	-41.759
3600	1003.915	2457.122	1649.224	2908.434	413.145	2866.307	-41.588
3700	1005.293	2484.647	1671.432	3008.896	411.614	2934.521	-41.427
3800	1006.570	2511.474	1693.187	3109.490	409.736	3002.720	-41.274
3900	1007.756	2537.636	1714.506	3210.207	407.551	3070.925	-41.130
4000	1008.858	2563.164	1735.404	3311.038	405.043	3139.323	-40.995
4100	1009.885	2588.088	1755.899	3411.976	402.176	3207.716	-40.866
4200	1010.842	2612.435	1776.004	3513.013	398.979	3276.175	-40.744
4300	1011.737	2636.232	1795.733	3614.142	395.437	3344.628	-40.628
4400	1012.574	2659.501	1815.101	3715.358	391.559	3413.256	-40.520
4500	1013.358	2682.265	1834.119	3816.655	387.358	3482.031	-40.418
4600	1014.094	2704.546	1852.800	3918.028	382.785	3550.908	-40.321
4700	1014.785	2726.362	1871.155	4019.473	377.853	3619.780	-40.229
4800	1015.435	2747.734	1889.196	4120.984	372.608	3688.862	-40.142
4900	1016.047	2768.678	1906.931	4222.558	366.979	3757.927	-40.059
5000	1016.623	2789.211	1924.372	4324.192	361.055	3827.292	-39.983

3.312. Hexacene



Other names: 2,3-Benzo-6,7-naphthoanthracene

Formula: $C_{26}H_{16}$

Mass: 328.405 g/mol

CAS Number: 258-31-1

Point Group: D_{2h}

Length: 18.94 Å

Width: 7.429 Å

Breadth: 3.882 Å

L/B Ratio: 2.549

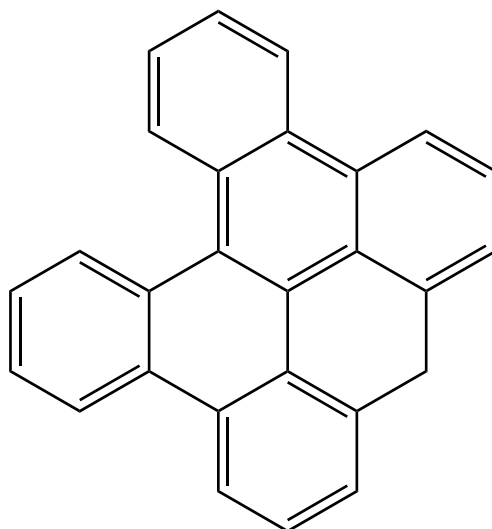
Cartesian coordinates:

C	-7.3015	0.7192	0.0000	C	1.2269	-1.4060	0.0000	H	-6.1294	-2.5034	0.0000
C	-7.3017	-0.7165	0.0000	C	1.2274	1.4056	0.0000	H	-6.1285	2.5057	0.0000
C	-6.1393	-1.4075	0.0000	C	2.4339	0.7158	0.0000	H	-3.6745	-2.5046	0.0000
C	-6.1388	1.4098	0.0000	C	2.4337	-0.7167	0.0000	H	-3.6736	2.5060	0.0000
C	-4.8691	0.7210	0.0000	C	3.6810	-1.4089	0.0000	H	-1.2248	-2.5027	0.0000
C	-4.8694	-0.7192	0.0000	C	3.6816	1.4075	0.0000	H	-1.2239	2.5032	0.0000
C	-3.6816	-1.4076	0.0000	C	4.8695	0.7191	0.0000	H	1.2240	-2.5032	0.0000
C	-3.6811	1.4089	0.0000	C	4.8692	-0.7210	0.0000	H	1.2249	2.5028	0.0000
C	-2.4335	0.7168	0.0000	C	6.1387	-1.4098	0.0000	H	3.6736	-2.5060	0.0000
C	-2.4338	-0.7159	0.0000	C	7.3015	-0.7192	0.0000	H	3.6746	2.5046	0.0000
C	-1.2276	-1.4056	0.0000	C	7.3018	0.7164	0.0000	H	6.1284	-2.5057	0.0000
C	-1.2270	1.4061	0.0000	C	6.1392	1.4075	0.0000	H	8.2658	-1.2376	0.0000
C	0.0002	0.7146	0.0000	H	-8.2659	1.2375	0.0000	H	8.2663	1.2345	0.0000
C	-0.0000	-0.7145	0.0000	H	-8.2663	-1.2345	0.0000	H	6.1294	2.5034	0.0000

Table 3.312: Table of thermodynamic data as a function of temperature for Hexacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-49.832	503.686	503.686	∞
100	109.137	339.743	770.334	-43.059	530.137	579.219	-302.547
200	215.412	446.160	581.659	-27.100	516.068	633.922	-165.560
250	277.173	500.817	559.998	-14.795	509.508	664.145	-138.763
298.15	337.204	554.784	554.784	0.000	503.686	694.471	-121.666
300	339.479	556.877	554.791	0.626	503.472	695.653	-121.121
350	399.234	613.743	559.145	19.109	498.117	728.119	-108.664
400	454.566	670.721	569.533	40.475	493.475	761.293	-99.413
450	504.668	727.206	583.921	64.478	489.462	795.016	-92.281
500	549.463	782.742	601.036	90.853	485.993	829.176	-86.622
600	624.681	889.840	640.326	149.708	480.388	898.369	-78.208
700	684.327	990.787	683.257	215.271	476.349	968.378	-72.260
800	732.316	1085.410	727.677	286.186	473.694	1038.854	-67.829
900	771.541	1174.004	772.401	361.443	472.249	1109.584	-64.397
1000	804.031	1257.027	816.757	440.271	471.847	1180.429	-61.658
1100	831.222	1334.972	860.361	522.073	472.293	1251.281	-59.417
1200	854.164	1408.309	902.998	606.374	473.444	1322.044	-57.546
1300	873.655	1477.470	944.554	692.791	475.119	1392.698	-55.958
1400	890.314	1542.840	984.975	781.011	477.187	1463.212	-54.592
1500	904.632	1604.766	1024.248	870.776	479.564	1533.569	-53.403
1600	917.001	1663.554	1062.384	961.872	482.122	1603.751	-52.356
1700	927.740	1719.476	1099.405	1054.122	484.788	1673.747	-51.427
1800	937.108	1772.776	1135.345	1147.375	487.487	1743.646	-50.598
1900	945.317	1823.667	1170.244	1241.505	490.187	1813.344	-49.851
2000	952.541	1872.343	1204.141	1336.405	492.833	1882.927	-49.176
2100	958.926	1918.976	1237.078	1431.985	495.351	1952.366	-48.561
2200	964.591	1963.718	1269.097	1528.167	497.738	2021.691	-48.000
2300	969.637	2006.709	1300.239	1624.883	499.989	2090.909	-47.485
2400	974.147	2048.074	1330.542	1722.076	502.034	2159.988	-47.010
2500	978.192	2087.924	1360.045	1819.697	503.884	2229.095	-46.573
2600	981.833	2126.361	1388.784	1917.701	505.505	2298.019	-46.167
2700	985.119	2163.479	1416.793	2016.051	506.899	2366.954	-45.791
2800	988.095	2199.360	1444.105	2114.714	508.042	2435.865	-45.441
2900	990.797	2234.081	1470.750	2213.661	508.905	2504.687	-45.113
3000	993.257	2267.713	1496.758	2312.866	509.530	2573.509	-44.808
3100	995.502	2300.319	1522.156	2412.305	509.841	2642.242	-44.521
3200	997.557	2331.958	1546.970	2511.960	509.880	2711.039	-44.252
3300	999.442	2362.683	1571.225	2611.811	509.627	2779.877	-44.001
3400	1001.174	2392.546	1594.945	2711.843	509.057	2848.645	-43.763
3500	1002.770	2421.591	1618.150	2812.041	508.173	2917.417	-43.539
3600	1004.243	2449.861	1640.862	2912.393	506.997	2986.301	-43.329
3700	1005.605	2477.395	1663.101	3012.886	505.498	3055.240	-43.131
3800	1006.868	2504.229	1684.884	3113.511	503.651	3124.164	-42.944
3900	1008.039	2530.398	1706.230	3214.257	501.495	3193.093	-42.766
4000	1009.129	2555.934	1727.155	3315.116	499.014	3262.215	-42.599
4100	1010.143	2580.864	1747.674	3416.080	496.174	3331.331	-42.441
4200	1011.090	2605.218	1767.803	3517.142	493.002	3400.512	-42.291
4300	1011.974	2629.020	1787.556	3618.296	489.484	3469.686	-42.147
4400	1012.801	2652.294	1806.945	3719.535	485.629	3539.035	-42.013
4500	1013.576	2675.063	1825.985	3820.854	481.450	3608.530	-41.886
4600	1014.303	2697.349	1844.686	3922.249	476.898	3678.127	-41.766
4700	1014.985	2719.170	1863.061	4023.713	471.987	3747.718	-41.650
4800	1015.628	2740.546	1881.120	4125.244	466.762	3817.519	-41.542
4900	1016.232	2761.493	1898.874	4226.838	461.151	3887.303	-41.438
5000	1016.802	2782.030	1916.332	4328.490	455.245	3957.386	-41.342

3.313. 8*H*-Tribenzo[*a,cd,l*]pyrene



Other names: [*Phenanthreno-9',10':9,10*]phenanthrene-1,1'*methylene*

Formula: C₂₇H₁₆

Mass: 340.416 g/mol

CAS Number: 190-61-4

Point Group: C₂

Length: 13.71 Å

Width: 12.75 Å

Breadth: 5.204 Å

L/B Ratio: 1.076

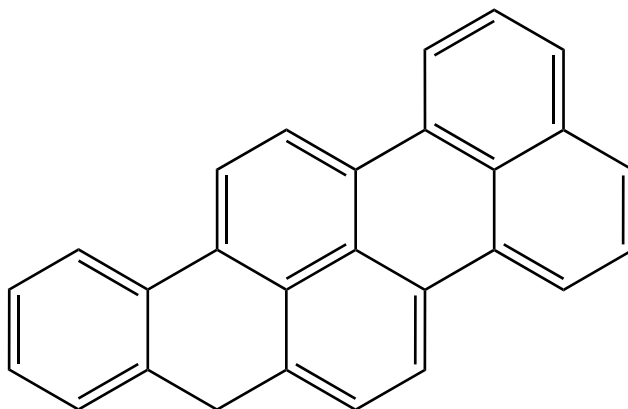
Cartesian coordinates:

C	2.5493	3.5578	-0.7489	C	-3.7454	2.8785	0.4877	H	4.7027	3.4014	-0.5785
C	1.3408	2.9131	-0.5997	C	-3.7043	1.5476	0.1393	H	2.4280	-4.4440	0.4485
C	3.7042	1.5475	-0.1395	C	-2.4592	-0.5658	-0.1945	H	4.5626	-3.2050	0.7182
C	3.7454	2.8786	-0.4878	C	-3.6502	-1.2800	-0.4262	H	4.5959	-0.7234	0.5098
C	2.4756	0.8656	-0.0206	C	-3.6351	-2.6538	-0.5327	H	-0.4158	3.4656	0.8135
C	1.2652	1.5663	-0.1835	C	-2.4315	-3.3498	-0.3887	H	-2.5788	4.6029	1.0745
C	2.4592	-0.5658	0.1944	C	-1.2378	-1.2557	-0.1064	H	-4.7027	3.4015	0.5785
C	2.4316	-3.3497	0.3887	C	-1.2450	-2.6663	-0.1713	H	-4.6365	0.9903	-0.0396
C	3.6352	-2.6537	0.5326	C	0.0000	-3.4632	0.0001	H	-4.5957	-0.7233	-0.5099
C	3.6502	-1.2799	0.4261	C	1.2451	-2.6662	0.1714	H	-4.5624	-3.2052	-0.7185
C	-0.0000	0.8706	0.0000	C	1.2378	-1.2557	0.1064	H	-2.4280	-4.4441	-0.4485
C	-2.4756	0.8656	0.0205	C	-0.0000	-0.5152	0.0000	H	0.1261	-4.1333	-0.8766
C	-1.2653	1.5662	0.1835	H	2.5786	4.6029	-1.0743	H	-0.1260	-4.1331	0.8770
C	-1.3409	2.9131	0.5999	H	0.4159	3.4660	-0.8133				
C	-2.5493	3.5578	0.7490	H	4.6366	0.9904	0.0394				

Table 3.313: Table of thermodynamic data as a function of temperature for 8*H*-Tribenzo[*a,cd,l*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-50.312	441.334	441.334	∞
100	109.931	349.066	783.605	-43.454	468.382	516.627	-269.853
200	217.371	456.567	593.225	-27.332	454.150	570.538	-149.006
250	279.439	511.685	571.379	-14.924	447.398	600.416	-125.447
298.15	340.363	566.119	566.119	0.000	441.334	630.451	-110.450
300	342.685	568.231	566.125	0.632	441.110	631.623	-109.973
350	403.924	625.697	570.524	19.311	435.480	663.833	-99.070
400	461.021	683.415	581.029	40.955	430.564	696.790	-90.990
450	512.943	740.766	595.597	65.326	426.292	730.329	-84.773
500	559.480	797.265	612.948	92.159	422.582	764.335	-79.848
600	637.721	906.467	652.846	152.173	416.558	833.282	-72.542
700	699.730	1009.609	696.520	219.162	412.173	903.111	-67.390
800	749.523	1106.412	741.772	291.713	409.232	973.451	-63.559
900	790.126	1197.116	787.381	368.762	407.544	1044.077	-60.595
1000	823.676	1282.155	832.652	449.503	406.933	1114.845	-58.232
1100	851.694	1362.013	877.183	533.313	407.192	1185.639	-56.300
1200	875.290	1437.160	920.748	619.695	408.174	1256.360	-54.687
1300	895.305	1508.033	963.224	708.252	409.689	1326.986	-53.318
1400	912.390	1575.024	1004.553	798.659	411.604	1397.485	-52.140
1500	927.057	1638.485	1044.719	890.649	413.833	1467.836	-51.114
1600	939.717	1698.730	1083.728	984.003	416.244	1538.023	-50.210
1700	950.699	1756.037	1121.603	1078.537	418.761	1608.032	-49.408
1800	960.273	1810.655	1158.379	1174.096	421.310	1677.955	-48.692
1900	968.658	1862.803	1194.092	1270.552	423.856	1747.684	-48.046
2000	976.033	1912.681	1228.783	1367.794	426.345	1817.306	-47.462
2100	982.549	1960.462	1262.496	1465.730	428.700	1886.793	-46.930
2200	988.328	2006.306	1295.270	1564.279	430.919	1956.173	-46.445
2300	993.474	2050.355	1327.149	1663.374	432.995	2025.455	-45.999
2400	998.072	2092.736	1358.171	1762.956	434.858	2094.603	-45.587
2500	1002.196	2133.564	1388.375	1862.973	436.520	2163.790	-45.209
2600	1005.906	2172.945	1417.798	1963.381	437.945	2232.798	-44.857
2700	1009.254	2210.972	1446.475	2064.142	439.135	2301.828	-44.531
2800	1012.286	2247.732	1474.438	2165.222	440.067	2370.842	-44.228
2900	1015.038	2283.303	1501.720	2266.590	440.709	2439.773	-43.944
3000	1017.543	2317.757	1528.350	2368.221	441.106	2508.712	-43.680
3100	1019.830	2351.160	1554.356	2470.091	441.181	2577.567	-43.431
3200	1021.922	2383.572	1579.765	2572.180	440.974	2646.498	-43.199
3300	1023.841	2415.048	1604.602	2674.470	440.467	2715.478	-42.982
3400	1025.604	2445.639	1628.891	2776.943	439.634	2784.393	-42.776
3500	1027.229	2475.393	1652.654	2879.586	438.477	2853.318	-42.583
3600	1028.728	2504.352	1675.911	2982.385	437.020	2922.368	-42.402
3700	1030.114	2532.557	1698.685	3085.328	435.231	2991.480	-42.231
3800	1031.399	2560.046	1720.992	3188.404	433.084	3060.584	-42.070
3900	1032.591	2586.852	1742.851	3291.605	430.619	3129.699	-41.917
4000	1033.700	2613.009	1764.279	3394.920	427.820	3199.019	-41.774
4100	1034.732	2638.547	1785.293	3498.342	424.653	3268.339	-41.638
4200	1035.695	2663.493	1805.907	3601.864	421.143	3337.732	-41.510
4300	1036.595	2687.874	1826.135	3705.479	417.278	3407.123	-41.387
4400	1037.436	2711.715	1845.992	3809.181	413.068	3476.700	-41.273
4500	1038.225	2735.038	1865.490	3912.965	408.524	3546.433	-41.165
4600	1038.964	2757.865	1884.642	4016.824	403.597	3616.277	-41.063
4700	1039.659	2780.217	1903.460	4120.756	398.300	3686.120	-40.966
4800	1040.312	2802.112	1921.955	4224.755	392.681	3756.185	-40.875
4900	1040.927	2823.569	1940.137	4328.817	386.665	3826.235	-40.787
5000	1041.506	2844.604	1958.017	4432.939	380.346	3896.599	-40.707

3.314. 9H-Naphtho[1,2,3-cd]perylene



Other names: 9H-Dibenzo[*de,rst*]pentaphene

Formula: C₂₇H₁₆

Mass: 340.416 g/mol

CAS Number: 188-77-2

Point Group: C_s

Length: 15.95 Å

Width: 9.172 Å

Breadth: 4.171 Å

L/B Ratio: 1.739

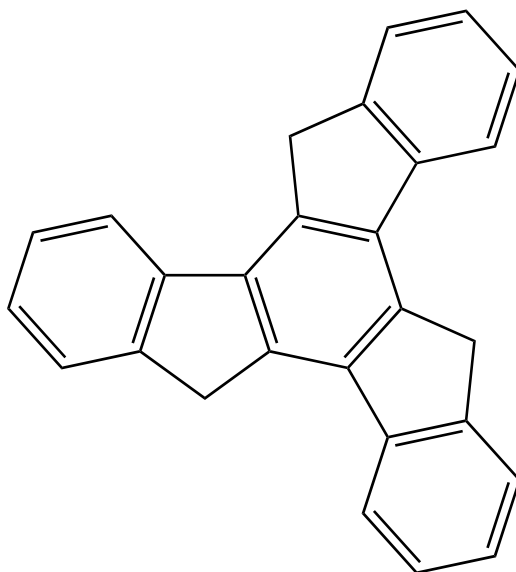
Cartesian coordinates:

C	5.7218	-1.5272	-0.0000	C	2.0366	-0.7664	0.0000	H	3.9089	-2.7036	-0.0000
C	6.2670	-0.2456	0.0000	C	1.1826	0.3773	0.0000	H	3.4584	2.5429	0.8858
C	5.4302	0.8605	0.0000	C	-2.5232	1.1677	-0.0000	H	3.4584	2.5429	-0.8858
C	4.3459	-1.6932	-0.0000	C	-3.3785	2.2506	-0.0000	H	1.2905	3.7970	0.0000
C	3.4882	-0.5843	0.0000	C	-4.7760	2.0708	-0.0000	H	-1.1727	3.4912	0.0000
C	4.0408	0.7019	0.0000	C	-5.3130	0.8111	0.0000	H	-0.3349	-3.2196	0.0000
C	3.1942	1.9272	0.0000	C	-2.2155	-1.2993	0.0000	H	2.1334	-2.9126	-0.0000
C	1.7228	1.6926	0.0000	C	-3.0634	-0.1523	0.0000	H	-2.9609	3.2692	-0.0000
C	0.8789	2.7812	0.0000	C	-4.4639	-0.3271	0.0000	H	-5.4248	2.9528	-0.0000
C	-0.5145	2.6085	0.0000	C	-5.0073	-1.6390	0.0000	H	-6.3987	0.6630	0.0000
C	-1.0728	1.3463	0.0000	C	-4.1773	-2.7282	0.0000	H	-6.0962	-1.7622	0.0000
C	-0.2209	0.2023	0.0000	C	-2.7786	-2.5592	0.0000	H	-4.5898	-3.7425	0.0000
C	-0.7660	-1.1162	0.0000	H	6.3791	-2.4026	-0.0000	H	-2.1234	-3.4439	0.0000
C	0.0858	-2.2020	0.0000	H	7.3535	-0.1117	0.0000				
C	1.4783	-2.0278	-0.0000	H	5.8568	1.8700	0.0000				

Table 3.314: Table of thermodynamic data as a function of temperature for 9*H*-Naphtho[1,2,3-*cd*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-50.724	434.881	434.881	∞
100	111.434	365.555	801.397	-43.584	461.798	508.395	-265.553
200	217.947	473.671	610.562	-27.378	447.650	560.618	-146.415
250	279.923	528.907	588.682	-14.944	440.925	589.637	-123.195
298.15	340.708	583.415	583.415	0.000	434.881	618.841	-108.416
300	343.023	585.530	583.422	0.632	434.658	619.981	-107.946
350	404.096	643.036	587.824	19.324	429.041	651.325	-97.203
400	461.043	700.766	598.335	40.973	424.129	683.414	-89.243
450	512.848	758.113	612.908	65.342	419.855	716.086	-83.119
500	559.305	814.597	630.261	92.168	416.138	749.225	-78.269
600	637.471	923.759	670.159	152.160	410.092	816.441	-71.076
700	699.478	1026.862	713.828	219.124	405.681	884.542	-66.004
800	749.298	1123.633	759.070	291.650	402.717	953.159	-62.234
900	789.939	1214.313	804.670	368.679	401.008	1022.064	-59.318
1000	823.527	1299.334	849.930	449.404	400.380	1091.113	-56.993
1100	851.577	1379.179	894.452	533.200	400.626	1160.191	-55.092
1200	875.201	1454.318	938.008	619.572	401.597	1229.195	-53.504
1300	895.238	1525.184	980.475	708.121	403.105	1298.106	-52.157
1400	912.339	1592.170	1021.798	798.522	405.014	1366.889	-50.998
1500	927.020	1655.628	1061.956	890.508	407.239	1435.527	-49.988
1600	939.690	1715.871	1100.959	983.859	409.646	1503.999	-49.100
1700	950.680	1773.177	1138.830	1078.390	412.162	1572.294	-48.310
1800	960.260	1827.794	1175.601	1173.948	414.708	1640.503	-47.605
1900	968.650	1879.942	1211.309	1270.403	417.254	1708.518	-46.969
2000	976.029	1929.819	1245.997	1367.644	419.743	1776.427	-46.395
2100	982.548	1977.601	1279.705	1465.580	422.097	1844.199	-45.871
2200	988.329	2023.445	1312.477	1564.129	424.316	1911.866	-45.393
2300	993.476	2067.494	1344.352	1663.224	426.392	1979.434	-44.953
2400	998.076	2109.874	1375.372	1762.806	428.256	2046.867	-44.548
2500	1002.200	2150.703	1405.574	1862.824	429.918	2114.341	-44.176
2600	1005.911	2190.084	1434.994	1963.233	431.343	2181.635	-43.829
2700	1009.260	2228.111	1463.669	2063.994	432.534	2248.952	-43.508
2800	1012.292	2264.871	1491.630	2165.074	433.466	2316.251	-43.209
2900	1015.044	2300.442	1518.910	2266.443	434.109	2383.468	-42.930
3000	1017.550	2334.897	1545.539	2368.075	434.507	2450.693	-42.669
3100	1019.836	2368.300	1571.543	2469.946	434.582	2517.835	-42.424
3200	1021.929	2400.712	1596.951	2572.035	434.376	2585.051	-42.196
3300	1023.847	2432.188	1621.787	2674.326	433.870	2652.317	-41.982
3400	1025.611	2462.780	1646.074	2776.800	433.037	2719.518	-41.779
3500	1027.235	2492.533	1669.835	2879.443	431.882	2786.729	-41.589
3600	1028.734	2521.493	1693.092	2982.243	430.425	2854.065	-41.411
3700	1030.121	2549.698	1715.864	3085.186	428.637	2921.463	-41.243
3800	1031.405	2577.187	1738.170	3188.263	426.490	2988.853	-41.084
3900	1032.597	2603.994	1760.029	3291.464	424.026	3056.253	-40.933
4000	1033.706	2630.151	1781.456	3394.780	421.227	3123.859	-40.793
4100	1034.738	2655.689	1802.469	3498.203	418.060	3191.465	-40.659
4200	1035.701	2680.635	1823.081	3601.725	414.552	3259.144	-40.533
4300	1036.600	2705.016	1843.309	3705.341	410.687	3326.821	-40.412
4400	1037.442	2728.857	1863.165	3809.043	406.477	3394.684	-40.299
4500	1038.230	2752.180	1882.663	3912.827	401.934	3462.702	-40.193
4600	1038.969	2775.008	1901.815	4016.688	397.007	3530.833	-40.093
4700	1039.664	2797.359	1920.632	4120.620	391.711	3598.961	-39.997
4800	1040.317	2819.255	1939.126	4224.619	386.092	3667.311	-39.908
4900	1040.931	2840.712	1957.307	4328.682	380.077	3735.648	-39.822
5000	1041.511	2861.747	1975.186	4432.804	373.759	3804.298	-39.742

3.315. Truxene



Other names: 10,15-Dihydrotribenzo[*a,f,k*]trindene
Triindeno[2,3:2',3':2''',3''''']benzene

Formula: C₂₇H₁₈
Mass: 342.432 g/mol
CAS Number: 548-35-6
Point Group: C_{3h}

Length: 14.35 Å
Width: 13.55 Å
Breadth: 4.182 Å
L/B Ratio: 1.059

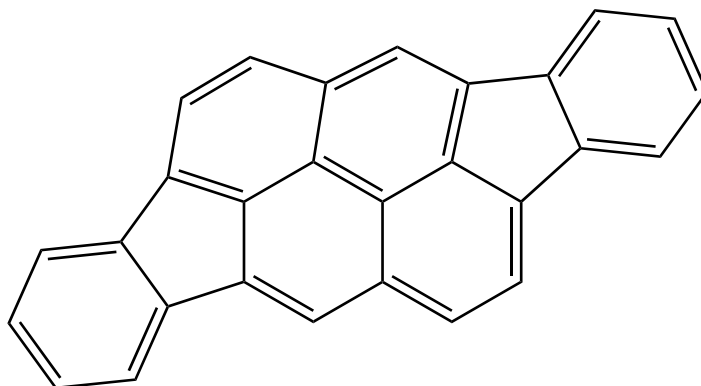
Cartesian coordinates:

C	-0.1807	1.3903	0.0000	C	-2.4401	-1.4654	0.0000	H	-3.0262	1.5078	0.8891
C	1.1334	0.8277	0.0000	C	-3.4099	-0.4344	0.0000	H	5.1240	-4.2084	-0.0000
C	2.1625	1.9212	0.0000	C	-4.7589	-0.7340	0.0000	H	5.8401	-1.8403	-0.0000
C	-1.1136	-0.8516	0.0000	C	-5.1417	-2.0780	-0.0000	H	4.1525	-0.0016	0.0000
C	-1.2835	0.5677	0.0000	C	-4.1906	-3.0913	-0.0000	H	2.7016	-4.8029	-0.0000
C	-2.7450	0.9123	0.0000	C	-2.8258	-2.7955	-0.0000	H	0.2063	-3.3743	0.8889
C	4.3704	-3.4141	-0.0000	C	-0.0490	2.8459	0.0000	H	0.2063	-3.3743	-0.8889
C	4.7725	-2.0837	-0.0000	C	1.3288	3.1703	0.0000	H	-5.5103	0.0614	0.0000
C	3.8340	-1.0496	0.0000	C	1.7439	4.4884	-0.0000	H	-6.2065	-2.3334	-0.0000
C	3.0150	-3.7545	-0.0000	C	0.7713	5.4919	-0.0000	H	-4.5135	-4.1376	-0.0000
C	2.0811	-2.7359	-0.0000	C	-0.5818	5.1749	-0.0000	H	-2.0775	-3.5955	-0.0000
C	2.4891	-1.3805	0.0000	C	-1.0080	3.8451	-0.0000	H	2.8085	4.7413	-0.0000
C	0.5825	-2.8333	0.0000	H	2.8191	1.8660	0.8890	H	1.0824	6.5418	-0.0000
C	0.1501	-1.3952	0.0000	H	2.8191	1.8660	-0.8890	H	-1.3264	5.9777	-0.0000
C	1.2943	-0.5385	0.0000	H	-3.0262	1.5078	-0.8891	H	-2.0749	3.5968	-0.0000

Table 3.315: Table of thermodynamic data as a function of temperature for Truxene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-52.804	404.362	404.362	∞
100	119.676	349.885	805.443	-45.556	434.775	493.012	-257.517
200	227.472	464.350	606.492	-28.428	418.855	557.569	-145.619
250	290.510	521.807	583.789	-15.495	411.232	593.129	-123.925
298.15	353.134	578.328	578.328	0.000	404.362	628.801	-110.161
300	355.530	580.520	578.335	0.656	404.109	630.192	-109.724
350	418.902	640.124	582.898	20.029	397.724	668.392	-99.750
400	478.174	699.985	593.793	42.477	392.155	707.439	-92.380
450	532.164	759.477	608.903	67.758	387.331	747.144	-86.724
500	580.615	818.102	626.901	95.600	383.170	787.372	-82.255
600	662.246	931.464	668.295	157.902	376.504	868.876	-75.641
700	727.182	1038.612	713.621	227.494	371.783	951.343	-70.989
800	779.540	1139.252	760.602	302.920	368.765	1034.351	-67.535
900	822.401	1233.625	807.974	383.086	367.220	1117.641	-64.865
1000	857.934	1322.169	855.012	467.157	366.934	1201.048	-62.735
1100	887.683	1405.375	901.302	554.480	367.669	1284.440	-60.992
1200	912.786	1483.720	946.604	644.539	369.248	1367.710	-59.534
1300	934.111	1557.647	990.791	736.912	371.459	1450.833	-58.294
1400	952.334	1627.556	1033.801	831.258	374.149	1533.770	-57.224
1500	967.990	1693.808	1075.612	927.293	377.214	1616.503	-56.290
1600	981.512	1756.722	1116.232	1024.785	380.512	1699.014	-55.466
1700	993.247	1816.587	1155.683	1123.536	383.953	1781.288	-54.731
1800	1003.481	1873.655	1193.997	1223.384	387.456	1863.423	-54.074
1900	1012.446	1928.156	1231.214	1324.190	390.981	1945.310	-53.479
2000	1020.334	1980.293	1267.374	1425.837	394.466	2027.038	-52.940
2100	1027.303	2030.247	1302.520	1528.226	397.828	2108.580	-52.447
2200	1033.485	2078.183	1336.695	1631.272	401.063	2189.970	-51.995
2300	1038.989	2124.247	1369.942	1734.901	404.162	2271.211	-51.580
2400	1043.909	2168.571	1402.301	1839.050	407.052	2352.275	-51.195
2500	1048.321	2211.277	1433.811	1943.666	409.743	2433.338	-50.841
2600	1052.290	2252.472	1464.510	2048.700	412.195	2514.179	-50.509
2700	1055.873	2292.254	1494.435	2154.111	414.412	2595.000	-50.202
2800	1059.117	2330.713	1523.619	2259.863	416.367	2675.772	-49.916
2900	1062.061	2367.931	1552.095	2365.924	418.028	2756.421	-49.647
3000	1064.742	2403.982	1579.893	2472.266	419.440	2837.043	-49.396
3100	1067.189	2438.935	1607.044	2578.865	420.522	2917.549	-49.159
3200	1069.428	2472.853	1633.573	2685.697	421.316	2998.097	-48.938
3300	1071.481	2505.793	1659.507	2792.744	421.803	3078.663	-48.730
3400	1073.368	2537.808	1684.871	2899.988	421.956	3159.135	-48.533
3500	1075.106	2568.948	1709.687	3007.413	421.777	3239.588	-48.347
3600	1076.710	2599.258	1733.978	3115.005	421.288	3320.135	-48.173
3700	1078.194	2628.779	1757.765	3222.751	420.458	3400.724	-48.009
3800	1079.569	2657.551	1781.067	3330.640	419.258	3481.272	-47.852
3900	1080.844	2685.610	1803.902	3438.661	417.731	3561.811	-47.704
4000	1082.031	2712.990	1826.288	3546.806	415.860	3642.529	-47.566
4100	1083.135	2739.721	1848.242	3655.065	413.608	3723.224	-47.433
4200	1084.166	2765.835	1869.780	3763.430	411.003	3803.970	-47.308
4300	1085.128	2791.357	1890.916	3871.896	408.031	3884.691	-47.189
4400	1086.029	2816.314	1911.666	3980.454	404.701	3965.580	-47.076
4500	1086.872	2840.730	1932.041	4089.099	401.027	4046.607	-46.971
4600	1087.664	2864.627	1952.056	4197.827	396.957	4127.722	-46.871
4700	1088.407	2888.027	1971.722	4306.630	392.505	4208.817	-46.775
4800	1089.106	2910.949	1991.051	4415.506	387.720	4290.116	-46.685
4900	1089.764	2933.412	2010.055	4524.450	382.525	4371.385	-46.599
5000	1090.384	2955.435	2028.743	4633.458	377.017	4452.954	-46.519

3.316. Diindeno[1,2,3-cd:1',d',3'-jk]pyrene



Formula: $C_{28}H_{14}$
Mass: 350.411 g/mol
CAS Number: 191-23-1
Point Group: C_{2h}

Length: 17.10 Å
Width: 9.874 Å
Breadth: 3.890 Å
L/B Ratio: 1.732

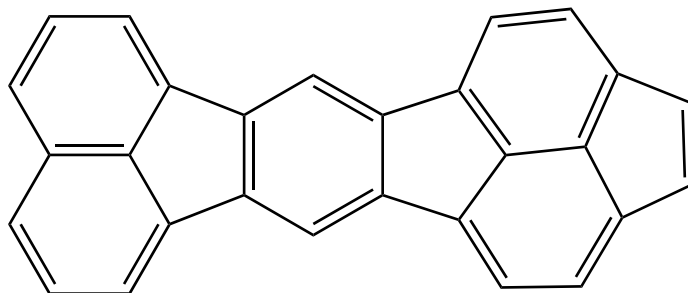
Cartesian coordinates:

C	-5.3121	-1.1574	0.0000	C	-0.8815	-2.9265	0.0000	H	-7.4043	-0.6263	0.0000
C	-4.0251	-0.6627	0.0000	C	-2.2641	-2.6682	0.0000	H	-6.9993	1.8122	0.0000
C	-3.7891	0.7553	0.0000	C	1.7693	0.3313	0.0000	H	-4.6756	2.7196	0.0000
C	-4.8477	1.6386	0.0000	C	2.7281	1.3579	0.0000	H	-5.4977	-2.2361	0.0000
C	-6.1500	1.1208	0.0000	C	2.2641	2.6682	0.0000	H	-1.9228	3.1137	0.0000
C	-6.3771	-0.2467	0.0000	C	0.8814	2.9265	0.0000	H	0.5422	3.9688	0.0000
C	-2.7281	-1.3579	0.0000	C	2.3364	-1.0032	0.0000	H	2.9714	3.5041	0.0000
C	-1.7693	-0.3313	0.0000	C	1.5239	-2.0940	0.0000	H	-0.5421	-3.9688	0.0000
C	-2.3363	1.0032	0.0000	C	3.7891	-0.7553	0.0000	H	-2.9716	-3.5039	0.0000
C	-0.4133	-0.5777	0.0000	C	4.0251	0.6627	0.0000	H	1.9228	-3.1137	0.0000
C	0.4133	0.5777	0.0000	C	5.3120	1.1574	0.0000	H	5.4975	2.2361	0.0000
C	-0.0801	1.9042	0.0000	C	6.3770	0.2467	0.0000	H	7.4043	0.6262	0.0000
C	-1.5239	2.0940	0.0000	C	6.1500	-1.1208	0.0000	H	6.9993	-1.8121	0.0000
C	0.0802	-1.9042	0.0000	C	4.8477	-1.6386	0.0000	H	4.6755	-2.7196	0.0000

Table 3.316: Table of thermodynamic data as a function of temperature for Diindeno[1,2,3-*cd*:1',*d'*,3'-*jk*]pyrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.389	520.001	520.001	∞
100	106.663	340.462	769.237	-42.877	543.147	582.276	-304.143
200	214.317	445.513	581.051	-27.108	530.931	626.265	-163.560
250	277.239	500.045	559.365	-14.830	525.149	650.765	-135.967
298.15	338.604	554.136	554.136	0.000	520.001	675.440	-118.332
300	340.933	556.237	554.142	0.629	519.810	676.402	-117.770
350	402.149	613.437	558.520	19.221	515.072	702.887	-104.898
400	458.880	670.897	568.976	40.768	510.964	729.996	-95.326
450	510.237	727.964	583.478	65.019	507.404	757.593	-87.937
500	556.106	784.145	600.744	91.700	504.307	785.582	-82.068
600	632.881	892.603	640.429	151.304	499.224	842.340	-73.331
700	693.373	994.885	683.837	217.734	495.444	899.848	-67.146
800	741.655	1090.741	728.775	289.573	492.824	957.802	-62.537
900	780.793	1180.433	774.031	365.761	491.214	1016.015	-58.967
1000	812.954	1264.415	818.916	445.499	490.480	1074.373	-56.118
1100	839.681	1343.190	863.034	528.171	490.447	1132.779	-53.790
1200	862.095	1417.241	906.164	613.292	490.994	1191.143	-51.848
1300	881.039	1487.014	948.187	700.475	491.958	1249.455	-50.203
1400	897.161	1552.912	989.050	789.406	493.221	1307.684	-48.789
1500	910.967	1615.292	1028.739	879.830	494.717	1365.817	-47.561
1600	922.857	1674.474	1067.264	971.536	496.325	1423.837	-46.483
1700	933.152	1730.738	1104.651	1064.348	497.984	1481.730	-45.527
1800	942.114	1784.335	1140.934	1158.122	499.624	1539.590	-44.677
1900	949.951	1835.487	1176.153	1252.734	501.219	1597.307	-43.912
2000	956.837	1884.392	1210.352	1348.080	502.724	1654.969	-43.222
2100	962.915	1931.226	1243.572	1444.074	504.064	1712.544	-42.596
2200	968.300	1976.148	1275.857	1540.640	505.241	1770.061	-42.026
2300	973.092	2019.298	1307.248	1637.714	506.254	1827.530	-41.504
2400	977.371	2060.805	1337.787	1735.241	507.034	1884.909	-41.023
2500	981.205	2100.782	1367.512	1833.174	507.596	1942.374	-40.583
2600	984.654	2139.334	1396.461	1931.470	507.906	1999.704	-40.174
2700	987.765	2176.554	1424.668	2030.093	507.970	2057.102	-39.796
2800	990.580	2212.529	1452.167	2129.013	507.762	2114.521	-39.446
2900	993.135	2247.335	1478.990	2228.200	507.256	2171.900	-39.119
3000	995.459	2281.043	1505.166	2327.632	506.497	2229.330	-38.815
3100	997.581	2313.719	1530.724	2427.286	505.406	2286.708	-38.530
3200	999.521	2345.422	1555.690	2527.142	504.029	2344.204	-38.264
3300	1001.300	2376.207	1580.090	2627.184	502.347	2401.788	-38.016
3400	1002.934	2406.123	1603.948	2727.397	500.332	2459.336	-37.782
3500	1004.440	2435.218	1627.284	2827.767	497.991	2516.931	-37.562
3600	1005.829	2463.534	1650.122	2928.281	495.346	2574.690	-37.357
3700	1007.113	2491.110	1672.480	3028.929	492.366	2632.538	-37.164
3800	1008.303	2517.984	1694.378	3129.701	489.026	2690.416	-36.982
3900	1009.407	2544.190	1715.834	3230.587	485.368	2748.329	-36.809
4000	1010.434	2569.759	1736.864	3331.580	481.374	2806.484	-36.648
4100	1011.390	2594.721	1757.484	3432.671	477.011	2864.668	-36.496
4200	1012.281	2619.104	1777.709	3533.855	472.306	2922.953	-36.351
4300	1013.114	2642.933	1797.555	3635.125	467.246	2981.263	-36.214
4400	1013.892	2666.233	1817.034	3736.476	461.840	3039.787	-36.086
4500	1014.622	2689.026	1836.159	3837.902	456.103	3098.493	-35.966
4600	1015.306	2711.334	1854.943	3939.399	449.982	3157.344	-35.852
4700	1015.949	2733.176	1873.397	4040.962	443.493	3216.214	-35.743
4800	1016.553	2754.572	1891.533	4142.587	436.681	3275.334	-35.642
4900	1017.122	2775.539	1909.361	4244.272	429.473	3334.460	-35.545
5000	1017.658	2796.093	1926.890	4346.011	421.964	3393.926	-35.455

3.317. Acenaphtho[1,2-*k*]cyclopenta[*cd*]fluoranthene



Formula: $C_{28}H_{14}$
Mass: 350.411 g/mol
CAS Number: 30909-04-7
Point Group: C_{2v}

Length: 16.61 Å
Width: 9.197 Å
Breadth: 3.887 Å
L/B Ratio: 1.806

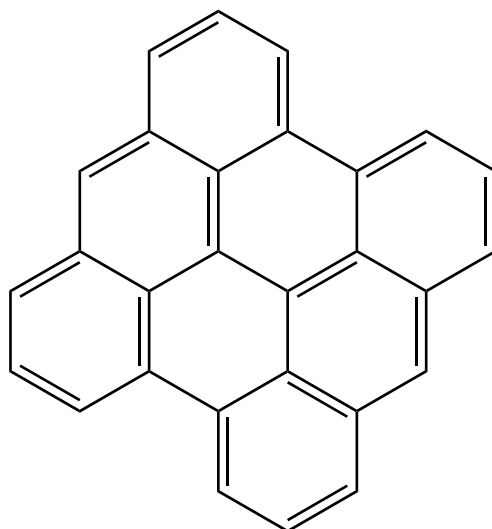
Cartesian coordinates:

C	6.3488	0.6841	0.0000	C	-1.6754	0.7128	0.0000	H	-6.9783	1.3372	0.0000
C	4.9573	1.1963	0.0000	C	-0.4900	1.4421	0.0000	H	-3.1317	3.3348	0.0000
C	4.1906	-0.0000	0.0000	C	-3.0679	-1.1812	0.0000	H	-5.6115	3.3986	0.0000
C	4.9573	-1.1963	0.0000	C	-3.8722	-0.0000	0.0000	H	-6.9783	-1.3372	0.0000
C	6.3488	-0.6841	0.0000	C	-3.0679	1.1812	0.0000	H	-5.6115	-3.3986	0.0000
C	2.8388	0.0000	0.0000	C	-3.6949	2.3964	0.0000	H	-3.1317	-3.3348	0.0000
C	2.0886	1.2079	0.0000	C	-5.1181	2.4203	0.0000	H	-0.4954	-2.5365	0.0000
C	2.8072	2.3804	0.0000	C	-5.8847	1.2793	0.0000	H	-0.4954	2.5365	0.0000
C	4.2502	2.3753	0.0000	C	-5.2603	-0.0000	0.0000	H	4.7668	3.3405	0.0000
C	2.0886	-1.2079	0.0000	C	-3.6949	-2.3964	0.0000	H	2.2955	3.3483	0.0000
C	0.6927	-0.7215	0.0000	C	-5.1181	-2.4203	0.0000	H	2.2955	-3.3483	0.0000
C	0.6927	0.7215	0.0000	C	-5.8847	-1.2793	0.0000	H	4.7668	-3.3405	0.0000
C	-0.4900	-1.4421	0.0000	C	4.2502	-2.3753	0.0000	H	7.2229	-1.3322	0.0000
C	-1.6754	-0.7128	0.0000	C	2.8072	-2.3804	0.0000	H	7.2229	1.3322	0.0000

Table 3.317: Table of thermodynamic data as a function of temperature for Acenaphtho[1,2-*k*]cyclopenta[*cd*]fluoranthene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.898	653.630	653.630	∞
100	108.204	345.844	777.853	-43.201	676.453	715.043	-373.492
200	215.784	451.748	588.290	-27.308	664.359	758.445	-198.082
250	279.322	506.674	566.442	-14.942	658.665	782.625	-163.517
298.15	341.133	561.173	561.173	0.000	653.630	806.970	-141.375
300	343.474	563.291	561.180	0.633	653.444	807.920	-140.668
350	404.914	620.902	565.589	19.359	648.839	834.041	-124.471
400	461.680	678.734	576.119	41.046	644.871	860.767	-112.402
450	512.950	736.128	590.716	65.435	641.449	887.964	-103.070
500	558.660	792.586	608.090	92.248	638.484	915.538	-95.644
600	635.044	901.476	647.995	152.088	633.637	971.429	-84.569
700	695.150	1004.062	691.612	218.715	630.054	1028.034	-76.711
800	743.100	1100.133	736.740	290.714	627.594	1085.059	-70.846
900	781.967	1189.979	782.164	367.033	626.115	1142.324	-66.297
1000	813.912	1274.074	827.196	446.878	625.487	1199.722	-62.666
1100	840.468	1352.931	871.443	529.637	625.541	1257.158	-59.696
1200	862.747	1427.044	914.687	614.829	626.160	1314.544	-57.219
1300	881.585	1496.865	956.810	702.071	627.183	1371.873	-55.121
1400	897.622	1562.800	997.763	791.053	628.496	1429.115	-53.320
1500	911.359	1625.210	1037.531	881.519	630.035	1486.258	-51.755
1600	923.193	1684.415	1076.127	973.261	631.680	1543.284	-50.382
1700	933.444	1740.698	1113.578	1066.105	633.370	1600.183	-49.167
1800	942.368	1794.311	1149.919	1159.906	635.036	1657.046	-48.085
1900	950.174	1845.476	1185.191	1254.541	636.656	1713.764	-47.114
2000	957.035	1894.392	1219.437	1349.909	638.182	1770.427	-46.238
2100	963.090	1941.235	1252.701	1445.922	639.540	1827.002	-45.443
2200	968.457	1986.164	1285.026	1542.504	640.734	1883.518	-44.719
2300	973.233	2029.321	1316.455	1639.593	641.762	1939.985	-44.058
2400	977.498	2070.834	1347.028	1737.134	642.555	1996.361	-43.449
2500	981.321	2110.816	1376.785	1835.078	643.130	2052.823	-42.890
2600	984.760	2149.372	1405.762	1933.385	643.451	2109.149	-42.372
2700	987.862	2186.596	1433.997	2032.019	643.525	2165.543	-41.894
2800	990.669	2222.574	1461.521	2130.948	643.326	2221.957	-41.450
2900	993.217	2257.383	1488.368	2230.144	642.829	2278.332	-41.036
3000	995.535	2291.095	1514.567	2329.584	642.077	2334.757	-40.651
3100	997.651	2323.773	1540.146	2429.244	640.994	2391.130	-40.289
3200	999.586	2355.478	1565.132	2529.108	639.623	2447.620	-39.952
3300	1001.361	2386.265	1589.551	2629.156	637.948	2504.198	-39.637
3400	1002.991	2416.183	1613.425	2729.375	635.939	2560.741	-39.340
3500	1004.493	2445.279	1636.779	2829.750	633.603	2617.330	-39.061
3600	1005.879	2473.596	1659.632	2930.270	630.963	2674.082	-38.799
3700	1007.160	2501.174	1682.006	3030.923	627.988	2730.925	-38.553
3800	1008.348	2528.049	1703.918	3131.699	624.653	2787.796	-38.320
3900	1009.449	2554.256	1725.387	3232.589	620.999	2844.702	-38.100
4000	1010.473	2579.826	1746.429	3333.586	617.010	2901.850	-37.893
4100	1011.427	2604.789	1767.062	3434.682	612.650	2959.027	-37.698
4200	1012.317	2629.173	1787.299	3535.869	607.949	3016.306	-37.512
4300	1013.147	2653.003	1807.156	3637.143	602.893	3073.609	-37.336
4400	1013.925	2676.304	1826.645	3738.497	597.490	3131.126	-37.170
4500	1014.652	2699.098	1845.781	3839.926	591.756	3188.825	-37.014
4600	1015.335	2721.406	1864.574	3941.426	585.638	3246.668	-36.866
4700	1015.976	2743.249	1883.038	4042.992	579.151	3304.531	-36.725
4800	1016.579	2764.645	1901.183	4144.620	572.343	3362.644	-36.592
4900	1017.147	2785.612	1919.019	4246.307	565.137	3420.763	-36.465
5000	1017.682	2806.167	1936.557	4348.048	557.630	3479.221	-36.346

3.318. Phenanthro[1,10,9,8-*opqra*]perylene



Other names: Bisanthrene
Dibenzo[*fg,op*]anthanthrene

Formula: C₂₈H₁₄
Mass: 350.411 g/mol
CAS Number: 190-39-6
Point Group: D_{2h}

Length: 13.76 Å
Width: 12.89 Å
Breadth: 3.889 Å
L/B Ratio: 1.067

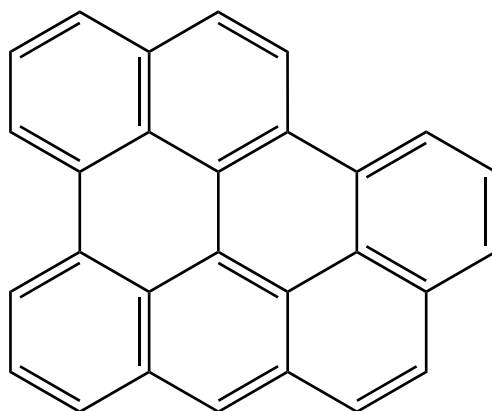
Cartesian coordinates:

C	3.3836	-3.1610	0.0000	C	2.5289	0.5184	0.0000	H	4.2923	-3.7719	0.0000
C	3.5130	-1.7492	0.0000	C	3.7575	1.1324	0.0000	H	4.5165	-1.2959	0.0000
C	2.1523	-3.7438	0.0000	C	3.8677	2.5458	0.0000	H	2.0435	-4.8343	0.0000
C	0.9695	-2.9387	0.0000	C	2.7522	3.3277	0.0000	H	-0.3917	-4.6183	0.0000
C	-0.2990	-3.5251	0.0000	C	1.3359	1.3172	0.0000	H	-4.6703	-0.5168	0.0000
C	-1.4506	-2.7335	0.0000	C	1.4507	2.7334	0.0000	H	-4.8663	-2.9951	0.0000
C	-3.7575	-1.1325	0.0000	C	0.2991	3.5252	0.0000	H	-2.8285	-4.4210	0.0000
C	-3.8676	-2.5460	0.0000	C	0.0612	0.7221	0.0000	H	4.6703	0.5166	0.0000
C	-2.7521	-3.3278	0.0000	C	-1.0950	1.5235	0.0000	H	4.8664	2.9949	0.0000
C	1.0949	-1.5235	0.0000	C	-0.9695	2.9388	0.0000	H	2.8286	4.4210	0.0000
C	2.4054	-0.9370	0.0000	C	-2.1522	3.7438	0.0000	H	0.3917	4.6183	0.0000
C	-0.0613	-0.7221	0.0000	C	-3.3835	3.1611	0.0000	H	-2.0435	4.8343	0.0000
C	-2.5289	-0.5184	0.0000	C	-3.5131	1.7493	0.0000	H	-4.2923	3.7721	0.0000
C	-1.3359	-1.3173	0.0000	C	-2.4055	0.9370	0.0000	H	-4.5165	1.2961	0.0000

Table 3.318: Table of thermodynamic data as a function of temperature for Phenanthro[1,10,9,8-*opqra*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-48.667	476.914	476.914	∞
100	101.727	331.088	754.981	-42.389	500.548	540.614	-282.382
200	212.407	433.848	568.505	-26.931	488.020	585.687	-152.963
250	275.491	487.981	546.953	-14.743	482.149	610.781	-127.613
298.15	336.714	541.754	541.754	0.000	476.914	636.044	-111.430
300	339.036	543.844	541.760	0.625	476.720	637.030	-110.914
350	400.099	600.739	546.114	19.119	471.882	664.142	-99.116
400	456.769	657.920	556.517	40.561	467.670	691.893	-90.350
450	508.151	714.739	570.946	64.707	464.005	720.145	-83.591
500	554.101	770.703	588.132	91.285	460.805	748.801	-78.225
600	631.107	878.816	627.649	150.700	455.533	806.921	-70.247
700	691.828	980.843	670.893	216.965	451.587	865.822	-64.607
800	740.302	1076.505	715.681	288.659	448.823	925.190	-60.407
900	779.596	1166.047	760.802	364.720	447.086	984.834	-57.157
1000	811.885	1249.910	805.565	444.345	446.239	1044.637	-54.565
1100	838.718	1328.588	849.574	526.916	446.104	1104.498	-52.447
1200	861.224	1402.559	892.605	611.945	446.560	1164.326	-50.681
1300	880.249	1472.266	934.539	699.045	447.440	1224.110	-49.184
1400	896.440	1538.108	975.322	787.900	448.628	1283.817	-47.899
1500	910.307	1600.441	1014.937	878.255	450.055	1343.433	-46.782
1600	922.252	1659.581	1053.395	969.898	451.601	1402.939	-45.800
1700	932.597	1715.810	1090.721	1062.652	453.201	1462.324	-44.931
1800	941.602	1769.377	1126.947	1156.373	454.787	1521.679	-44.157
1900	949.479	1820.502	1162.115	1250.935	456.334	1580.892	-43.461
2000	956.401	1869.384	1196.266	1346.237	457.793	1640.054	-42.833
2100	962.510	1916.198	1229.441	1442.188	459.091	1699.131	-42.263
2200	967.924	1961.101	1261.685	1538.715	460.229	1758.152	-41.743
2300	972.741	2004.235	1293.038	1635.753	461.206	1817.127	-41.267
2400	977.044	2045.727	1323.541	1733.247	461.952	1876.012	-40.829
2500	980.900	2085.692	1353.233	1831.147	462.483	1934.986	-40.428
2600	984.368	2124.232	1382.150	1929.414	462.763	1993.825	-40.056
2700	987.497	2161.442	1410.328	2028.009	462.799	2052.734	-39.712
2800	990.328	2197.407	1437.799	2126.903	462.566	2111.664	-39.393
2900	992.898	2232.205	1464.596	2226.066	462.035	2170.557	-39.095
3000	995.236	2265.905	1490.747	2325.475	461.253	2229.499	-38.818
3100	997.370	2298.574	1516.282	2425.107	460.141	2288.392	-38.558
3200	999.322	2330.271	1541.226	2524.943	458.743	2347.402	-38.317
3300	1001.111	2361.049	1565.605	2624.966	457.042	2406.502	-38.091
3400	1002.756	2390.960	1589.443	2725.160	455.008	2465.566	-37.878
3500	1004.270	2420.050	1612.761	2825.513	452.649	2524.678	-37.678
3600	1005.668	2448.361	1635.580	2926.010	449.988	2583.953	-37.491
3700	1006.960	2475.933	1657.922	3026.643	446.993	2643.320	-37.316
3800	1008.157	2502.803	1679.803	3127.399	443.638	2702.715	-37.151
3900	1009.269	2529.005	1701.243	3228.271	439.965	2762.146	-36.994
4000	1010.301	2554.571	1722.258	3329.250	435.958	2821.820	-36.848
4100	1011.263	2579.530	1742.864	3430.329	431.582	2881.522	-36.710
4200	1012.160	2603.909	1763.076	3531.501	426.865	2941.327	-36.580
4300	1012.998	2627.736	1782.908	3632.759	421.793	3001.157	-36.456
4400	1013.782	2651.033	1802.375	3734.099	416.375	3061.201	-36.340
4500	1014.516	2673.824	1821.488	3835.514	410.628	3121.427	-36.232
4600	1015.204	2696.130	1840.260	3937.000	404.496	3181.797	-36.130
4700	1015.851	2717.970	1858.703	4038.553	397.997	3242.188	-36.032
4800	1016.459	2739.364	1876.828	4140.169	391.176	3302.829	-35.941
4900	1017.031	2760.328	1894.646	4241.844	383.959	3363.476	-35.854
5000	1017.571	2780.880	1912.166	4343.574	376.440	3424.463	-35.774

3.319. Benzo[*cd*]naphtho[3,2,1,8-*pqra*]perylene



Other names: Naphtho[8,1,2-*efg*]anthanthrene
Phenaleno[12,3,4-*ghij*]perylene

Formula: C₂₈H₁₄
Mass: 350.411 g/mol
CAS Number: 6208-20-4
Point Group: C_s

Length: 13.77 Å
Width: 11.65 Å
Breadth: 3.889 Å
L/B Ratio: 1.182

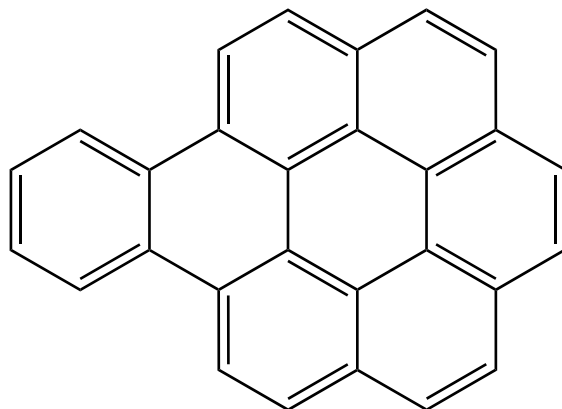
Cartesian coordinates:

C	4.0762	1.6446	0.0000	C	1.3505	0.8695	0.0000	H	5.1396	1.9107	0.0000
C	3.1214	2.5967	0.0000	C	0.0025	0.5032	0.0000	H	3.3844	3.6609	0.0000
C	1.7164	2.2512	0.0000	C	-1.0071	1.5057	0.0000	H	1.0132	4.2846	0.0000
C	0.7388	3.2224	0.0000	C	-2.3893	1.1541	0.0000	H	-1.3467	4.9211	0.0000
C	-0.6339	2.8682	0.0000	C	-2.7642	-0.2571	0.0000	H	-3.7479	4.2776	0.0000
C	-1.6430	3.8660	0.0000	C	-4.0927	-0.6465	0.0000	H	-4.4090	1.8790	0.0000
C	-2.9669	3.5100	0.0000	C	-4.4453	-2.0051	0.0000	H	2.7599	-3.5341	0.0000
C	-3.3427	2.1533	0.0000	C	-3.4729	-2.9767	0.0000	H	5.1549	-2.8548	0.0000
C	3.7351	0.2395	0.0000	C	-1.7462	-1.2512	0.0000	H	5.7804	-0.4523	0.0000
C	3.0399	-2.4695	0.0000	C	-2.1066	-2.6137	0.0000	H	-4.8773	0.1261	0.0000
C	4.3706	-2.0905	0.0000	C	-1.0818	-3.6077	0.0000	H	-5.5047	-2.2821	0.0000
C	4.7234	-0.7416	0.0000	C	0.2313	-3.2493	0.0000	H	-3.7434	-4.0386	0.0000
C	2.0189	-1.5056	0.0000	C	0.6212	-1.8770	0.0000	H	-1.3751	-4.6637	0.0000
C	2.3701	-0.1385	0.0000	C	-0.3614	-0.8893	0.0000	H	1.0283	-4.0089	0.0000

Table 3.319: Table of thermodynamic data as a function of temperature for Benzo[*cd*]naphtho[3,2,1,8-*pgra*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-47.996	414.466	414.466	∞
100	99.422	337.678	756.827	-41.915	438.575	477.982	-249.667
200	209.978	438.747	572.255	-26.702	425.802	522.489	-136.457
250	273.158	492.348	550.878	-14.632	419.812	547.353	-114.361
298.15	334.446	545.716	545.716	0.000	414.466	572.415	-100.283
300	336.770	547.792	545.722	0.621	414.268	573.393	-99.835
350	397.889	604.342	550.049	19.003	409.319	600.317	-89.591
400	454.625	661.232	560.391	40.336	404.997	627.895	-81.993
450	506.092	717.804	574.744	64.377	401.227	655.988	-76.144
500	552.142	773.556	591.846	90.855	397.927	684.497	-71.507
600	629.374	881.331	631.190	150.085	392.470	742.349	-64.626
700	690.322	983.108	674.269	216.187	388.362	801.011	-59.771
800	739.003	1078.583	718.906	287.742	385.458	860.163	-56.162
900	778.475	1167.982	763.891	363.682	383.600	919.607	-53.371
1000	810.915	1251.736	808.533	443.203	382.649	979.221	-51.148
1100	837.875	1330.327	852.434	525.683	382.424	1038.905	-49.332
1200	860.487	1404.229	895.368	610.633	382.800	1098.563	-47.818
1300	879.600	1473.881	937.216	697.664	383.612	1158.182	-46.535
1400	895.866	1539.677	977.921	786.458	384.738	1217.730	-45.433
1500	909.796	1601.973	1017.467	876.759	386.111	1277.191	-44.475
1600	921.795	1661.082	1055.861	968.353	387.608	1336.546	-43.633
1700	932.186	1717.285	1093.129	1061.065	389.166	1395.782	-42.886
1800	941.231	1770.829	1129.304	1154.746	390.713	1454.990	-42.222
1900	949.142	1821.935	1164.423	1249.273	392.224	1514.060	-41.624
2000	956.094	1870.801	1198.529	1344.542	393.651	1573.078	-41.084
2100	962.229	1917.600	1231.664	1440.465	394.920	1632.015	-40.593
2200	967.667	1962.491	1263.871	1536.965	396.031	1690.896	-40.146
2300	972.504	2005.614	1295.189	1633.978	396.983	1749.732	-39.737
2400	976.825	2047.097	1325.660	1731.448	397.707	1808.480	-39.360
2500	980.697	2087.052	1355.321	1829.328	398.216	1867.318	-39.015
2600	984.180	2125.585	1384.210	1927.575	398.477	1926.021	-38.693
2700	987.322	2162.788	1412.361	2026.153	398.495	1984.795	-38.397
2800	990.165	2198.747	1439.808	2125.029	398.244	2043.591	-38.123
2900	992.745	2233.539	1466.582	2224.177	397.698	2102.350	-37.867
3000	995.093	2267.235	1492.711	2323.571	396.901	2161.159	-37.628
3100	997.236	2299.899	1518.225	2423.189	395.775	2219.919	-37.405
3200	999.195	2331.592	1543.150	2523.012	394.364	2278.797	-37.197
3300	1000.992	2362.366	1567.511	2623.022	392.650	2337.765	-37.003
3400	1002.643	2392.274	1591.331	2723.205	390.605	2396.698	-36.820
3500	1004.164	2421.360	1614.633	2823.547	388.236	2455.678	-36.648
3600	1005.567	2449.668	1637.437	2924.034	385.564	2514.823	-36.488
3700	1006.865	2477.238	1659.763	3024.656	382.559	2574.059	-36.338
3800	1008.067	2504.105	1681.631	3125.404	379.195	2633.324	-36.197
3900	1009.182	2530.305	1703.057	3226.267	375.513	2692.625	-36.063
4000	1010.219	2555.868	1724.059	3327.238	371.498	2752.168	-35.939
4100	1011.185	2580.825	1744.653	3428.308	367.114	2811.741	-35.821
4200	1012.085	2605.203	1764.853	3529.473	362.389	2871.417	-35.711
4300	1012.927	2629.028	1784.674	3630.724	357.310	2931.117	-35.605
4400	1013.713	2652.324	1804.129	3732.056	351.885	2991.032	-35.507
4500	1014.450	2675.113	1823.232	3833.465	346.131	3051.129	-35.416
4600	1015.142	2697.418	1841.995	3934.945	339.993	3111.371	-35.330
4700	1015.791	2719.256	1860.428	4036.492	333.488	3171.633	-35.248
4800	1016.401	2740.649	1878.544	4138.101	326.661	3232.145	-35.172
4900	1016.976	2761.612	1896.353	4239.771	319.438	3292.664	-35.100
5000	1017.518	2782.163	1913.864	4341.496	311.914	3353.522	-35.033

3.320. Benzo[*a*]coronene



Formula: C₂₈H₁₄
Mass: 350.411 g/mol
CAS Number: 190-70-5
Point Group: C_{2v}

Length: 14.10 Å
Width: 11.65 Å
Breadth: 3.885 Å
L/B Ratio: 1.210

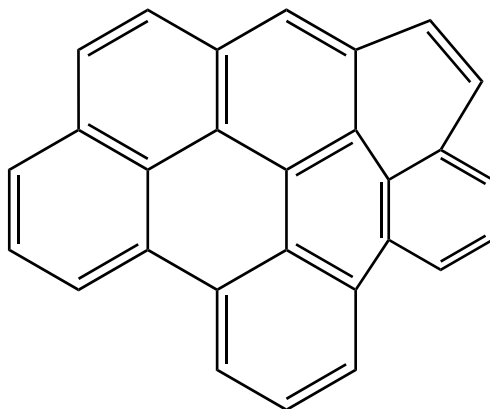
Cartesian coordinates:

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C	-5.3333	-0.6438	0.0000	C	-1.5838	2.8637	0.0000	H	-6.2901	-1.1758	0.0000
C	-4.1484	-1.3451	0.0000	C	-1.6318	1.4458	0.0000	H	-4.1479	-2.4460	0.0000
C	-4.1185	1.4343	0.0000	C	-0.4348	0.7245	0.0000	H	-4.0943	2.5349	0.0000
C	-2.8933	0.7348	0.0000	C	-0.4503	-0.7149	0.0000	H	5.4006	-1.2993	0.0000
C	-2.9085	-0.6722	0.0000	C	-1.6626	-1.4101	0.0000	H	5.4274	1.1826	0.0000
C	4.4630	-0.7318	0.0000	C	-1.6453	-2.8288	0.0000	H	4.2263	3.3274	0.0000
C	4.4777	0.6352	0.0000	C	-0.4665	-3.5250	0.0000	H	2.0926	4.5967	0.0000
C	2.0417	0.6906	0.0000	C	0.7790	-1.4350	0.0000	H	-0.3670	4.6300	0.0000
C	3.2638	1.3760	0.0000	C	0.7740	-2.8388	0.0000	H	-2.5374	3.4141	0.0000
C	3.2630	2.8048	0.0000	C	2.0166	-3.5450	0.0000	H	-2.6106	-3.3584	0.0000
C	2.0928	3.5006	0.0000	C	3.2016	-2.8746	0.0000	H	-0.4670	-4.6209	0.0000
C	0.8098	1.4178	0.0000	C	3.2334	-1.4461	0.0000	H	1.9928	-4.6408	0.0000
C	0.8352	2.8214	0.0000	C	2.0263	-0.7345	0.0000	H	4.1534	-3.4180	0.0000

Table 3.320: Table of thermodynamic data as a function of temperature for Benzo[*a*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-47.943	381.741	381.741	∞
100	99.236	331.310	749.989	-41.868	405.897	445.940	-232.930
200	209.733	432.164	565.593	-26.686	393.093	491.096	-128.258
250	273.002	485.722	544.226	-14.626	387.092	516.290	-107.871
298.15	334.340	539.067	539.067	0.000	381.741	541.672	-94.897
300	336.666	541.142	539.073	0.621	381.542	542.663	-94.484
350	397.818	597.678	543.398	18.998	376.589	569.919	-85.054
400	454.580	654.560	553.739	40.329	372.264	597.831	-78.067
450	506.068	711.129	568.089	64.368	368.492	626.257	-72.693
500	552.137	766.879	585.189	90.845	365.192	655.099	-68.436
600	629.395	874.656	624.529	150.076	359.735	713.620	-62.125
700	690.360	976.437	667.607	216.181	355.631	772.949	-57.677
800	739.049	1071.918	712.243	287.740	352.730	832.767	-54.373
900	778.525	1161.323	757.228	363.685	350.878	892.878	-51.820
1000	810.967	1245.082	801.871	443.211	349.931	953.158	-49.787
1100	837.926	1323.678	845.772	525.696	349.712	1013.507	-48.126
1200	860.536	1397.585	888.708	610.651	350.093	1073.829	-46.742
1300	879.647	1467.240	930.558	697.687	350.909	1134.113	-45.568
1400	895.910	1533.040	971.264	786.486	352.041	1194.324	-44.560
1500	909.838	1595.338	1010.811	876.791	353.418	1254.449	-43.683
1600	921.834	1654.450	1049.207	968.389	354.919	1314.467	-42.912
1700	932.222	1710.655	1086.476	1061.104	356.480	1374.367	-42.228
1800	941.265	1764.201	1122.652	1154.789	358.031	1434.237	-41.620
1900	949.174	1815.309	1157.773	1249.320	359.545	1493.970	-41.071
2000	956.123	1864.176	1191.880	1344.592	360.975	1553.651	-40.576
2100	962.257	1910.977	1225.017	1440.517	362.247	1613.250	-40.127
2200	967.692	1955.869	1257.224	1537.020	363.360	1672.793	-39.716
2300	972.528	1998.994	1288.543	1634.035	364.315	1732.292	-39.341
2400	976.848	2040.477	1319.015	1731.508	365.041	1791.702	-38.995
2500	980.719	2080.434	1348.678	1829.390	365.553	1851.201	-38.678
2600	984.200	2118.967	1377.568	1927.639	365.816	1910.566	-38.383
2700	987.340	2156.171	1405.720	2026.219	365.835	1970.002	-38.111
2800	990.182	2192.131	1433.167	2125.097	365.587	2029.460	-37.859
2900	992.761	2226.923	1459.942	2224.246	365.042	2088.880	-37.624
3000	995.109	2260.619	1486.072	2323.642	364.246	2148.351	-37.405
3100	997.250	2293.284	1511.587	2423.261	363.122	2207.773	-37.200
3200	999.209	2324.977	1536.513	2523.086	361.712	2267.312	-37.009
3300	1001.005	2355.752	1560.874	2623.098	360.000	2326.941	-36.832
3400	1002.656	2385.660	1584.695	2723.282	357.956	2386.535	-36.664
3500	1004.176	2414.747	1607.997	2823.624	355.588	2446.177	-36.506
3600	1005.579	2443.055	1630.802	2924.113	352.918	2505.983	-36.360
3700	1006.876	2470.625	1653.129	3024.737	349.913	2565.880	-36.223
3800	1008.077	2497.493	1674.997	3125.485	346.551	2625.807	-36.093
3900	1009.192	2523.693	1696.424	3226.349	342.870	2685.769	-35.971
4000	1010.229	2549.256	1717.426	3327.321	338.855	2745.974	-35.858
4100	1011.194	2574.214	1738.020	3428.393	334.472	2806.208	-35.751
4200	1012.094	2598.592	1758.221	3529.558	329.748	2866.544	-35.650
4300	1012.935	2622.417	1778.043	3630.809	324.670	2926.906	-35.554
4400	1013.721	2645.713	1797.499	3732.143	319.246	2987.481	-35.465
4500	1014.458	2668.502	1816.602	3833.552	313.493	3048.240	-35.382
4600	1015.149	2690.807	1835.365	3935.033	307.355	3109.143	-35.305
4700	1015.798	2712.646	1853.799	4036.580	300.851	3170.066	-35.231
4800	1016.408	2734.038	1871.915	4138.191	294.025	3231.239	-35.162
4900	1016.983	2755.002	1889.724	4239.861	286.802	3292.419	-35.097
5000	1017.524	2775.553	1907.236	4341.586	279.279	3353.938	-35.038

3.321. Phenanthro[5,4,3,2-*abcde*]perylene



Other names: Dibenzo[*cd,fg*]anthanthrene

Formula: C₂₈H₁₄

Mass: 350.411 g/mol

CAS Number: 75449-92-2

Point Group: C_{2v}

Length: 14.11 Å

Width: 11.66 Å

Breadth: 3.885 Å

L/B Ratio: 1.211

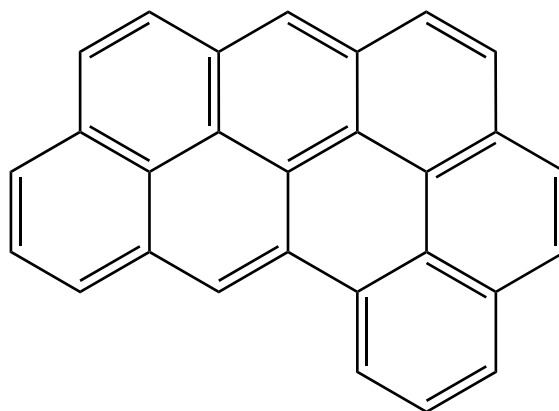
Cartesian coordinates:

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C	-2.4767	3.0730	0.0000	C	1.2151	0.9631	0.0000	H	-2.4551	4.1689	0.0000
C	-3.6801	0.9594	0.0000	C	3.6762	0.9742	0.0000	H	-5.8397	0.8186	0.0000
C	-4.8959	0.2617	0.0000	C	2.4638	0.2530	0.0000	H	-5.8530	-1.6661	0.0000
C	-4.9018	-1.1234	0.0000	C	2.4837	-1.1609	0.0000	H	-3.7130	-2.9367	0.0000
C	-3.7048	-1.8358	0.0000	C	3.7122	-1.8209	0.0000	H	-0.0084	4.1644	0.0000
C	-1.2173	2.3724	0.0000	C	4.9063	-1.1038	0.0000	H	4.5947	2.9522	0.0000
C	-0.0061	3.0674	0.0000	C	4.8948	0.2814	0.0000	H	2.4383	4.1787	0.0000
C	-2.4648	0.2431	0.0000	C	0.0024	-1.1895	0.0000	H	3.7247	-2.9218	0.0000
C	-2.4790	-1.1709	0.0000	C	-1.2178	-1.8996	0.0000	H	5.8597	-1.6425	0.0000
C	-1.2189	0.9582	0.0000	C	-1.1969	-3.2976	0.0000	H	5.8364	0.8419	0.0000
C	1.2078	2.3772	0.0000	C	0.0080	-3.9869	0.0000	H	-2.1532	-3.8430	0.0000
C	3.6396	2.4144	0.0000	C	1.2101	-3.2929	0.0000	H	0.0101	-5.0818	0.0000
C	2.4643	3.0829	0.0000	C	1.2254	-1.8947	0.0000	H	2.1687	-3.8343	0.0000

Table 3.321: Table of thermodynamic data as a function of temperature for Phenanthro[5,4,3,2-*abcde*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-48.049	401.398	401.398	∞
100	99.557	331.885	751.558	-41.967	425.454	465.440	-243.116
200	210.268	433.100	566.760	-26.732	412.704	510.520	-133.331
250	273.468	486.769	545.359	-14.648	406.728	535.664	-111.919
298.15	334.768	540.192	540.192	0.000	401.398	560.994	-98.282
300	337.093	542.270	540.199	0.621	401.200	561.982	-97.848
350	398.224	598.871	544.529	19.020	396.267	589.180	-87.929
400	454.968	655.806	554.880	40.370	391.963	617.031	-80.574
450	506.438	712.419	569.245	64.428	388.210	645.394	-74.914
500	552.484	768.207	586.360	90.923	384.927	674.171	-70.429
600	629.696	876.043	625.732	150.187	379.503	732.555	-63.773
700	690.615	977.867	668.839	216.320	375.426	791.744	-59.079
800	739.264	1073.379	713.502	287.902	372.549	851.417	-55.591
900	778.708	1162.807	758.511	363.867	370.716	911.380	-52.894
1000	811.122	1246.584	803.175	443.410	369.787	971.511	-50.745
1100	838.060	1325.194	847.095	525.909	369.582	1031.709	-48.991
1200	860.652	1399.112	890.048	610.877	369.976	1091.879	-47.527
1300	879.748	1468.776	931.912	697.923	370.803	1152.010	-46.287
1400	896.000	1534.583	972.631	786.732	371.944	1212.067	-45.222
1500	909.917	1596.887	1012.190	877.045	373.329	1272.038	-44.295
1600	921.904	1656.004	1050.597	968.651	374.838	1331.901	-43.481
1700	932.285	1712.213	1087.876	1061.373	376.405	1391.644	-42.759
1800	941.322	1765.762	1124.060	1155.063	377.962	1451.359	-42.116
1900	949.225	1816.873	1159.189	1249.599	379.482	1510.935	-41.538
2000	956.170	1865.743	1193.304	1344.876	380.917	1570.460	-41.015
2100	962.299	1912.546	1226.447	1440.806	382.193	1629.902	-40.541
2200	967.731	1957.440	1258.661	1537.313	383.311	1689.289	-40.108
2300	972.564	2000.566	1289.986	1634.332	384.269	1748.630	-39.712
2400	976.881	2042.051	1320.464	1731.809	384.998	1807.883	-39.347
2500	980.749	2082.009	1350.131	1829.694	385.513	1867.224	-39.013
2600	984.228	2120.543	1379.026	1927.946	385.779	1926.432	-38.702
2700	987.367	2157.748	1407.182	2026.528	385.802	1985.710	-38.415
2800	990.207	2193.709	1434.634	2125.409	385.556	2045.010	-38.149
2900	992.785	2228.502	1461.412	2224.561	385.013	2104.273	-37.901
3000	995.130	2262.199	1487.546	2323.958	384.220	2163.586	-37.671
3100	997.271	2294.865	1513.065	2423.580	383.098	2222.849	-37.454
3200	999.228	2326.558	1537.994	2523.406	381.690	2282.231	-37.253
3300	1001.023	2357.334	1562.358	2623.420	379.980	2341.702	-37.065
3400	1002.673	2387.242	1586.182	2723.606	377.938	2401.138	-36.888
3500	1004.192	2416.329	1609.486	2823.950	375.571	2460.621	-36.722
3600	1005.594	2444.638	1632.294	2924.441	372.902	2520.269	-36.567
3700	1006.890	2472.208	1654.623	3025.066	369.899	2580.008	-36.422
3800	1008.091	2499.077	1676.494	3125.815	366.538	2639.776	-36.285
3900	1009.205	2525.277	1697.923	3226.681	362.859	2699.579	-36.156
4000	1010.241	2550.841	1718.927	3327.654	358.846	2759.626	-36.036
4100	1011.206	2575.798	1739.524	3428.727	354.463	2819.702	-35.923
4200	1012.105	2600.177	1759.726	3529.893	349.741	2879.880	-35.816
4300	1012.946	2624.002	1779.550	3631.146	344.664	2940.082	-35.714
4400	1013.732	2647.298	1799.007	3732.480	339.241	3000.500	-35.620
4500	1014.468	2670.088	1818.113	3833.891	333.488	3061.099	-35.532
4600	1015.158	2692.393	1836.877	3935.372	327.352	3121.844	-35.449
4700	1015.807	2714.232	1855.313	4036.921	320.849	3182.608	-35.370
4800	1016.417	2735.625	1873.430	4138.532	314.023	3243.623	-35.297
4900	1016.991	2756.588	1891.241	4240.203	306.802	3304.644	-35.227
5000	1017.532	2777.140	1908.754	4341.929	299.279	3366.005	-35.164

3.322. Benzo[*lmn*]naphtho[2,1,8-*gra*]perylene



Other names: Dibenzo[*cd,hi*]anthanthrene

Formula: C₂₈H₁₄

Mass: 350.411 g/mol

CAS Number: 75449-94-4

Point Group: C_s

Length: 14.27 Å

Width: 11.11 Å

Breadth: 3.887 Å

L/B Ratio: 1.285

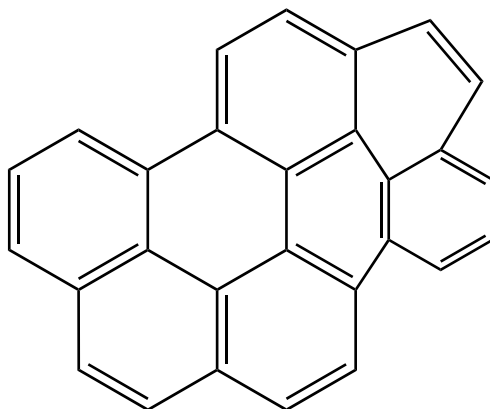
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C	1.9069	-2.0606	0.0000	C	2.4585	1.6580	0.0000	H	1.0610	-4.0410	0.0000
C	0.8614	-2.9623	0.0000	C	2.7241	0.2718	0.0000	H	-3.6913	-3.7054	0.0000
C	-0.4784	-2.5100	0.0000	C	4.0635	-0.1931	0.0000	H	-1.3422	-4.5068	0.0000
C	-2.8571	-2.9945	0.0000	C	5.1066	0.7262	0.0000	H	-5.8142	0.5585	0.0000
C	-1.5678	-3.4342	0.0000	C	4.8367	2.0977	0.0000	H	-5.3115	-1.8735	0.0000
C	-3.1522	-1.5987	0.0000	C	3.5356	2.5635	0.0000	H	0.8993	3.1915	0.0000
C	-4.7788	0.1988	0.0000	C	-3.7241	1.1674	0.0000	H	6.1446	0.3750	0.0000
C	-4.5039	-1.1325	0.0000	C	-2.3849	0.7314	0.0000	H	5.6701	2.8083	0.0000
C	-2.1060	-0.6739	0.0000	C	-1.3308	1.6839	0.0000	H	3.3326	3.6404	0.0000
C	-0.7502	-1.1288	0.0000	C	-1.6417	3.0346	0.0000	H	-0.8239	3.7718	0.0000
C	0.0568	1.2241	0.0000	C	-2.9762	3.4649	0.0000	H	-3.1917	4.5385	0.0000
C	0.3165	-0.1923	0.0000	C	-4.0053	2.5507	0.0000	H	-5.0488	2.8853	0.0000

Table 3.322: Table of thermodynamic data as a function of temperature for Benzo[*lmn*]naphtho[2,1,8-*qra*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K_f</i>
0	0.0	0.0	∞	-48.105	407.332	407.332	∞
100	99.392	337.793	758.186	-42.039	431.316	470.712	-245.869
200	210.662	439.022	573.015	-26.799	418.571	515.203	-134.554
250	274.175	492.815	551.560	-14.686	412.624	540.048	-112.834
298.15	335.641	546.379	546.379	0.000	407.332	565.083	-98.998
300	337.969	548.462	546.385	0.623	407.136	566.060	-98.558
350	399.157	605.203	550.727	19.067	402.249	592.945	-88.490
400	455.891	662.263	561.103	40.464	397.991	620.476	-81.024
450	507.319	718.982	575.500	64.567	394.283	648.514	-75.276
500	553.313	774.861	592.651	91.105	391.043	676.960	-70.720
600	630.422	882.838	632.095	150.446	385.697	734.671	-63.958
700	691.262	984.768	675.272	216.648	381.688	793.175	-59.186
800	739.854	1080.363	719.999	288.291	378.873	852.154	-55.639
900	779.251	1169.858	765.066	364.313	377.097	911.415	-52.896
1000	811.627	1253.690	809.782	443.908	376.220	970.838	-50.710
1100	838.530	1332.346	853.750	526.456	376.063	1030.323	-48.925
1200	861.089	1406.303	896.745	611.469	376.502	1089.776	-47.436
1300	880.155	1476.001	938.649	698.558	377.372	1149.186	-46.174
1400	896.378	1541.837	979.404	787.406	378.552	1208.519	-45.089
1500	910.269	1604.167	1018.996	877.756	379.974	1267.763	-44.147
1600	922.232	1663.305	1057.433	969.395	381.516	1326.897	-43.318
1700	932.590	1719.533	1094.740	1062.149	383.116	1385.909	-42.583
1800	941.604	1773.100	1130.950	1155.869	384.701	1444.891	-41.929
1900	949.488	1824.226	1166.103	1250.432	386.249	1503.733	-41.340
2000	956.415	1873.108	1200.241	1345.734	387.709	1562.522	-40.808
2100	962.528	1919.922	1233.404	1441.688	389.009	1621.227	-40.325
2200	967.945	1964.827	1265.637	1538.217	390.149	1679.875	-39.884
2300	972.764	2007.962	1296.981	1635.257	391.128	1738.477	-39.481
2400	977.068	2049.455	1327.475	1732.753	391.876	1796.990	-39.110
2500	980.925	2089.421	1357.158	1830.656	392.410	1855.590	-38.770
2600	984.393	2127.962	1386.068	1928.925	392.692	1914.057	-38.453
2700	987.522	2165.173	1414.238	2027.523	392.731	1972.593	-38.161
2800	990.353	2201.139	1441.703	2126.419	392.500	2031.150	-37.891
2900	992.922	2235.937	1468.494	2225.585	391.972	2089.669	-37.638
3000	995.260	2269.639	1494.640	2324.996	391.192	2148.238	-37.403
3100	997.394	2302.309	1520.170	2424.630	390.082	2206.758	-37.183
3200	999.345	2334.006	1545.109	2524.469	388.686	2265.394	-36.978
3300	1001.134	2364.785	1569.484	2624.494	386.988	2324.121	-36.787
3400	1002.778	2394.697	1593.317	2724.690	384.956	2382.811	-36.607
3500	1004.291	2423.787	1616.631	2825.045	382.600	2441.549	-36.437
3600	1005.688	2452.098	1639.447	2925.545	379.941	2500.451	-36.280
3700	1006.980	2479.671	1661.785	3026.179	376.947	2559.444	-36.132
3800	1008.177	2506.542	1683.663	3126.938	373.594	2618.465	-35.993
3900	1009.287	2532.744	1705.100	3227.812	369.923	2677.522	-35.861
4000	1010.319	2558.310	1726.112	3328.793	365.918	2736.822	-35.738
4100	1011.280	2583.269	1746.715	3429.873	361.544	2796.151	-35.623
4200	1012.177	2607.650	1766.924	3531.046	356.828	2855.582	-35.514
4300	1013.014	2631.477	1786.754	3632.306	351.758	2915.037	-35.410
4400	1013.797	2654.774	1806.218	3733.647	346.342	2974.707	-35.314
4500	1014.531	2677.566	1825.329	3835.064	340.596	3034.559	-35.224
4600	1015.219	2699.871	1844.099	3936.552	334.466	3094.556	-35.139
4700	1015.865	2721.712	1862.540	4038.107	327.968	3154.572	-35.058
4800	1016.473	2743.106	1880.663	4139.724	321.149	3214.839	-34.984
4900	1017.045	2764.071	1898.479	4241.400	313.933	3275.112	-34.912
5000	1017.584	2784.623	1915.997	4343.132	306.415	3335.724	-34.847

3.323. Benzo[*pqr*]naphtho[8,1,2-*bcd*]perylene



Other names: Dibenzo[*hi,qr*]anthanthrene

Formula: C₂₈H₁₄

Mass: 350.411 g/mol

CAS Number: 190-71-6

Point Group: C_{2h}

Length: 13.80 Å

Width: 10.40 Å

Breadth: 3.888 Å

L/B Ratio: 1.326

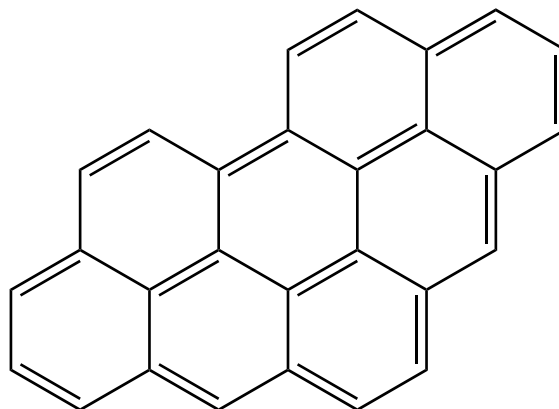
Cartesian coordinates:

C	4.4678	-2.1227	0.0000	C	1.0756	3.3605	0.0000	H	5.2066	-2.9310	0.0000
C	4.8852	-0.8039	0.0000	C	-0.2691	3.0667	0.0000	H	5.9539	-0.5613	0.0000
C	3.1087	-2.4353	0.0000	C	-0.7232	1.7326	0.0000	H	2.7804	-3.4861	0.0000
C	2.1463	-1.4286	0.0000	C	0.2126	0.6895	0.0000	H	-2.7806	3.4862	0.0000
C	-2.1464	1.4286	0.0000	C	0.7232	-1.7325	0.0000	H	-5.2067	2.9309	0.0000
C	-3.1088	2.4353	0.0000	C	-0.2126	-0.6894	0.0000	H	-5.9539	0.5612	0.0000
C	-4.4679	2.1226	0.0000	C	-1.0755	-3.3604	0.0000	H	5.4261	1.8295	0.0000
C	-4.8853	0.8038	0.0000	C	0.2691	-3.0666	0.0000	H	3.7518	3.6628	0.0000
C	2.5639	-0.0755	0.0000	C	-2.0308	-2.3254	0.0000	H	1.4139	4.4029	0.0000
C	3.9402	0.2345	0.0000	C	-1.5990	-0.9870	0.0000	H	-1.0193	3.8728	0.0000
C	4.3518	1.6122	0.0000	C	-2.5639	0.0755	0.0000	H	-1.4138	-4.4029	0.0000
C	3.4386	2.6125	0.0000	C	-3.9402	-0.2345	0.0000	H	1.0194	-3.8727	0.0000
C	1.5990	0.9871	0.0000	C	-4.3518	-1.6123	0.0000	H	-5.4261	-1.8297	0.0000
C	2.0308	2.3254	0.0000	C	-3.4386	-2.6125	0.0000	H	-3.7518	-3.6629	0.0000

Table 3.323: Table of thermodynamic data as a function of temperature for Benzo[*pqr*]naphtho[8,1,2-*bcd*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.116	392.721	392.721	∞
100	99.748	333.819	753.584	-41.976	416.769	456.562	-238.478
200	210.262	435.039	568.747	-26.742	404.018	501.446	-130.962
250	273.570	488.719	547.337	-14.655	398.045	526.493	-110.002
298.15	334.954	542.167	542.167	0.000	392.721	551.729	-96.659
300	337.282	544.247	542.174	0.622	392.524	552.713	-96.234
350	398.467	600.881	546.507	19.031	387.602	579.812	-86.530
400	455.242	657.850	556.864	40.394	383.311	607.561	-79.338
450	506.724	714.496	571.238	64.466	379.572	635.821	-73.803
500	552.772	770.315	588.363	90.976	376.303	664.493	-69.418
600	629.969	878.202	627.756	150.267	370.908	722.664	-62.912
700	690.865	980.067	670.886	216.427	366.857	781.635	-58.325
800	739.490	1075.611	715.570	288.033	364.004	841.087	-54.916
900	778.911	1165.064	760.599	364.019	362.192	900.825	-52.281
1000	811.305	1248.861	805.280	443.581	361.283	960.729	-50.182
1100	838.224	1327.488	849.217	526.098	361.094	1020.698	-48.468
1200	860.800	1401.419	892.184	611.082	361.504	1080.639	-47.038
1300	879.882	1471.094	934.062	698.142	362.345	1140.538	-45.826
1400	896.121	1536.911	974.794	786.963	363.499	1200.363	-44.785
1500	910.028	1599.223	1014.364	877.288	364.896	1260.100	-43.880
1600	922.005	1658.347	1052.781	968.905	366.415	1319.729	-43.084
1700	932.378	1714.562	1090.070	1061.636	367.992	1379.238	-42.378
1800	941.406	1768.116	1126.263	1155.336	369.558	1438.718	-41.750
1900	949.303	1819.232	1161.400	1249.880	371.086	1498.058	-41.184
2000	956.242	1868.105	1195.523	1345.164	372.529	1557.347	-40.673
2100	962.366	1914.911	1228.673	1441.101	373.811	1616.553	-40.209
2200	967.793	1959.808	1260.893	1537.614	374.935	1675.703	-39.785
2300	972.621	2002.937	1292.224	1634.639	375.900	1734.807	-39.398
2400	976.934	2044.424	1322.707	1732.121	376.635	1793.822	-39.041
2500	980.799	2084.384	1352.380	1830.011	377.155	1852.927	-38.714
2600	984.274	2122.921	1381.279	1928.268	377.425	1911.897	-38.410
2700	987.410	2160.127	1409.440	2026.855	377.452	1970.937	-38.129
2800	990.247	2196.089	1436.896	2125.740	377.210	2029.999	-37.869
2900	992.823	2230.884	1463.679	2224.896	376.672	2089.023	-37.627
3000	995.166	2264.582	1489.817	2324.297	375.882	2148.098	-37.401
3100	997.304	2297.249	1515.339	2423.922	374.763	2207.123	-37.189
3200	999.260	2328.944	1540.271	2523.752	373.359	2266.266	-36.992
3300	1001.053	2359.720	1564.639	2623.769	371.652	2325.499	-36.809
3400	1002.701	2389.630	1588.466	2723.958	369.613	2384.696	-36.636
3500	1004.219	2418.718	1611.773	2824.305	367.249	2443.941	-36.473
3600	1005.619	2447.027	1634.583	2924.797	364.583	2503.349	-36.322
3700	1006.914	2474.598	1656.916	3025.425	361.582	2562.849	-36.180
3800	1008.114	2501.467	1678.789	3126.177	358.223	2622.378	-36.046
3900	1009.227	2527.668	1700.220	3227.045	354.546	2681.943	-35.920
4000	1010.262	2553.232	1721.227	3328.020	350.535	2741.750	-35.803
4100	1011.226	2578.190	1741.826	3429.095	346.155	2801.587	-35.692
4200	1012.125	2602.569	1762.030	3530.263	341.434	2861.526	-35.588
4300	1012.964	2626.395	1781.856	3631.518	336.359	2921.489	-35.488
4400	1013.749	2649.692	1801.316	3732.854	330.938	2981.667	-35.396
4500	1014.485	2672.482	1820.423	3834.266	325.187	3042.028	-35.310
4600	1015.175	2694.787	1839.189	3935.749	319.053	3102.533	-35.230
4700	1015.822	2716.626	1857.626	4037.300	312.551	3163.058	-35.153
4800	1016.432	2738.019	1875.746	4138.913	305.727	3223.833	-35.082
4900	1017.005	2758.983	1893.558	4240.585	298.507	3284.615	-35.014
5000	1017.546	2779.535	1911.072	4342.312	290.986	3345.736	-34.952

3.324. Phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene



Other names: Naphtho[2,1,8-*hij*]anthanthrene

Formula: C₂₈H₁₄

Mass: 350.411 g/mol

CAS Number: 4552-79-8

Point Group: C_{2v}

Length: 15.85 Å

Width: 10.45 Å

Breadth: 3.885 Å

L/B Ratio: 1.517

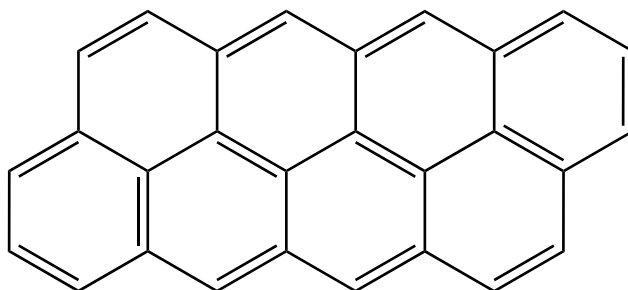
Cartesian coordinates:

C	4.9459	-1.4686	0.0000	C	1.4589	-2.7280	0.0000	H	5.5029	-2.4123	0.0000
C	5.6295	-0.2560	0.0000	C	2.8112	-2.7248	0.0000	H	6.7247	-0.2536	0.0000
C	4.9399	0.9474	0.0000	C	3.5500	-1.4883	0.0000	H	5.4887	1.8960	0.0000
C	3.5379	0.9602	0.0000	C	2.8349	-0.2673	0.0000	H	3.3663	3.1335	0.0000
C	2.8038	2.1916	0.0000	C	-3.5339	0.9749	0.0000	H	1.2461	4.3714	0.0000
C	1.4381	2.1944	0.0000	C	-4.9359	0.9680	0.0000	H	-1.2279	4.3766	0.0000
C	0.6798	3.4327	0.0000	C	-5.6305	-0.2325	0.0000	H	-3.3532	3.1475	0.0000
C	-0.6655	3.4355	0.0000	C	-4.9519	-1.4480	0.0000	H	0.8895	-3.6705	0.0000
C	-1.4289	2.2004	0.0000	C	-2.8360	-0.2555	0.0000	H	3.3776	-3.6632	0.0000
C	-2.7946	2.2033	0.0000	C	-3.5561	-1.4736	0.0000	H	-5.4807	1.9188	0.0000
C	-0.7005	0.9550	0.0000	C	-2.8225	-2.7131	0.0000	H	-6.7257	-0.2256	0.0000
C	0.7045	0.9521	0.0000	C	-1.4702	-2.7219	0.0000	H	-5.5129	-2.3893	0.0000
C	1.4038	-0.2745	0.0000	C	-0.7070	-1.5003	0.0000	H	-3.3928	-3.6491	0.0000
C	0.7008	-1.5033	0.0000	C	-1.4049	-0.2686	0.0000	H	-0.9048	-3.6667	0.0000

Table 3.324: Table of thermodynamic data as a function of temperature for Phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-48.042	424.499	424.499	∞
100	98.635	329.340	750.071	-42.073	448.450	488.691	-255.261
200	210.919	430.378	564.649	-26.854	435.683	534.043	-139.475
250	274.766	484.267	543.146	-14.720	429.757	559.319	-116.861
298.15	336.435	537.954	537.954	0.000	424.499	584.763	-102.446
300	338.770	540.042	537.960	0.625	424.305	585.755	-101.987
350	400.064	596.915	542.312	19.111	419.461	613.058	-91.492
400	456.834	654.099	552.712	40.555	415.249	641.000	-83.704
450	508.251	710.929	567.140	64.705	411.588	669.443	-77.705
500	554.208	766.904	584.327	91.289	408.394	698.289	-72.948
600	631.210	875.036	623.846	150.714	403.132	756.789	-65.883
700	691.937	977.079	667.095	216.989	399.197	816.066	-60.894
800	740.427	1072.757	711.888	288.695	396.444	875.810	-57.183
900	779.739	1162.314	757.015	364.769	394.721	935.828	-54.313
1000	812.045	1246.194	801.784	444.410	393.889	996.003	-52.025
1100	838.889	1324.888	845.799	526.997	393.771	1056.236	-50.155
1200	861.402	1398.874	888.837	612.044	394.244	1116.433	-48.596
1300	880.428	1468.595	930.778	699.161	395.142	1176.584	-47.275
1400	896.618	1534.450	971.568	788.035	396.348	1236.658	-46.139
1500	910.481	1596.795	1011.190	878.407	397.793	1296.639	-45.152
1600	922.421	1655.947	1049.655	970.067	399.355	1356.510	-44.285
1700	932.759	1712.186	1086.987	1062.838	400.972	1416.257	-43.515
1800	941.757	1765.761	1123.220	1156.574	402.574	1475.974	-42.831
1900	949.626	1816.895	1158.394	1251.152	404.136	1535.549	-42.214
2000	956.541	1865.784	1192.550	1346.468	405.610	1595.070	-41.658
2100	962.643	1912.604	1225.731	1442.433	406.921	1654.508	-41.153
2200	968.050	1957.514	1257.981	1538.973	408.072	1713.887	-40.692
2300	972.861	2000.654	1289.339	1636.023	409.062	1773.220	-40.270
2400	977.157	2042.151	1319.847	1733.528	409.819	1832.464	-39.882
2500	981.007	2082.120	1349.544	1831.440	410.361	1891.795	-39.526
2600	984.469	2120.664	1378.465	1929.717	410.652	1950.991	-39.195
2700	987.593	2157.878	1406.647	2028.322	410.698	2010.257	-38.890
2800	990.419	2193.846	1434.123	2127.225	410.474	2069.543	-38.607
2900	992.984	2228.647	1460.923	2226.397	409.952	2128.792	-38.343
3000	995.318	2262.350	1487.079	2325.814	409.178	2188.090	-38.097
3100	997.448	2295.022	1512.617	2425.454	408.074	2247.338	-37.867
3200	999.396	2326.721	1537.565	2525.298	406.683	2306.703	-37.652
3300	1001.182	2357.501	1561.948	2625.328	404.989	2366.158	-37.452
3400	1002.823	2387.414	1585.788	2725.529	402.963	2425.577	-37.264
3500	1004.334	2416.506	1609.109	2825.888	400.611	2485.043	-37.086
3600	1005.729	2444.819	1631.932	2926.392	397.956	2544.673	-36.921
3700	1007.018	2472.392	1654.276	3027.031	394.966	2604.393	-36.767
3800	1008.213	2499.264	1676.161	3127.793	391.617	2664.143	-36.620
3900	1009.322	2525.467	1697.603	3228.670	387.950	2723.928	-36.482
4000	1010.352	2551.034	1718.621	3329.655	383.948	2783.955	-36.354
4100	1011.312	2575.994	1739.229	3430.738	379.577	2844.011	-36.232
4200	1012.207	2600.375	1759.443	3531.915	374.864	2904.170	-36.118
4300	1013.043	2624.203	1779.278	3633.178	369.797	2964.352	-36.009
4400	1013.824	2647.501	1798.747	3734.521	364.384	3024.749	-35.908
4500	1014.557	2670.293	1817.862	3835.941	358.640	3085.329	-35.813
4600	1015.244	2692.600	1836.636	3937.431	352.513	3146.053	-35.724
4700	1015.889	2714.441	1855.082	4038.988	346.018	3206.796	-35.639
4800	1016.496	2735.835	1873.208	4140.608	339.200	3267.790	-35.560
4900	1017.067	2756.800	1891.028	4242.286	331.986	3328.790	-35.485
5000	1017.605	2777.353	1908.549	4344.020	324.471	3390.129	-35.416

3.325. peri-Naphthacenonaphthacene



Other names: Dibenzo[*cd,lm*]anthanthrene
Naphthaceno[4,5,6,7,8-*defghij*]naphthacene

Formula: C₂₈H₁₄

Mass: 350.411 g/mol

CAS Number: 180-50-1

Point Group: C_{2h}

Length: 15.28 Å

Width: 9.547 Å

Breadth: 3.886 Å

L/B Ratio: 1.601

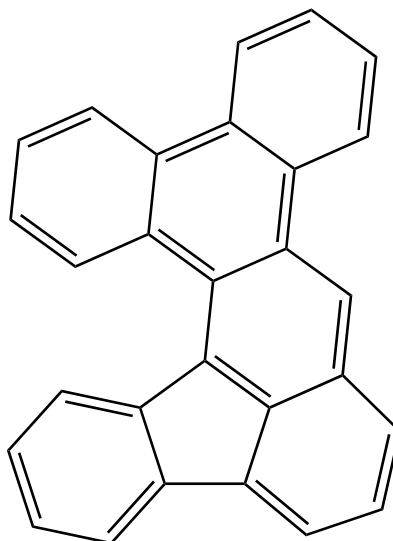
Cartesian coordinates:

C	5.4874	-0.2734	0.0000	C	-3.0768	-0.0079	0.0000	H	6.3784	-0.9113	0.0000
C	5.6403	1.1285	0.0000	C	-3.2340	-1.4143	0.0000	H	6.6512	1.5500	0.0000
C	4.5477	1.9562	0.0000	C	-2.0931	-2.2464	0.0000	H	4.6708	3.0452	0.0000
C	3.2340	1.4143	0.0000	C	-1.7780	0.5552	0.0000	H	2.2265	3.3352	0.0000
C	2.0930	2.2464	0.0000	C	-0.6553	-0.2825	0.0000	H	-0.2173	3.6217	0.0000
C	0.8185	1.7022	0.0000	C	-0.8184	-1.7021	0.0000	H	-2.6603	3.9020	0.0000
C	-0.3534	2.5331	0.0000	C	0.3534	-2.5331	0.0000	H	-4.9267	2.9056	0.0000
C	-1.6057	1.9882	0.0000	C	0.6553	0.2825	0.0000	H	-6.3785	0.9111	0.0000
C	-2.7987	2.8145	0.0000	C	1.7780	-0.5552	0.0000	H	-6.6512	-1.5499	0.0000
C	-4.0316	2.2728	0.0000	C	1.6057	-1.9882	0.0000	H	-4.6706	-3.0452	0.0000
C	-4.2281	0.8363	0.0000	C	2.7987	-2.8145	0.0000	H	-2.2263	-3.3353	0.0000
C	-5.4873	0.2734	0.0000	C	4.0315	-2.2728	0.0000	H	0.2174	-3.6217	0.0000
C	-5.6403	-1.1286	0.0000	C	4.2281	-0.8363	0.0000	H	2.6603	-3.9020	0.0000
C	-4.5477	-1.9562	0.0000	C	3.0768	0.0079	0.0000	H	4.9267	-2.9056	0.0000

Table 3.325: Table of thermodynamic data as a function of temperature for peri-Naphthacenonaphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-48.342	443.159	443.159	∞
100	99.483	332.423	755.233	-42.281	466.902	506.834	-264.737
200	211.978	434.068	568.934	-26.973	454.224	551.846	-144.124
250	275.998	488.213	547.338	-14.781	448.356	576.930	-120.540
298.15	337.736	542.125	542.125	0.000	443.159	602.179	-105.497
300	340.072	544.221	542.131	0.627	442.967	603.164	-105.018
350	401.353	601.295	546.498	19.179	438.188	630.252	-94.058
400	458.062	658.647	556.933	40.686	434.039	657.971	-85.920
450	509.397	715.617	571.406	64.895	430.438	686.183	-79.648
500	555.267	771.708	588.641	91.534	427.299	714.792	-74.672
600	632.112	880.019	628.257	151.057	422.135	772.801	-67.277
700	692.714	982.191	671.597	217.415	418.283	831.574	-62.052
800	741.109	1077.966	716.473	289.194	415.603	890.801	-58.162
900	780.346	1167.599	761.674	365.333	413.944	950.295	-55.153
1000	812.590	1251.540	806.509	445.031	413.170	1009.938	-52.753
1100	839.383	1330.283	850.583	527.670	413.104	1069.633	-50.792
1200	861.851	1404.310	893.674	612.764	413.623	1129.289	-49.156
1300	880.838	1474.065	935.662	699.924	414.565	1188.895	-47.769
1400	896.993	1539.949	976.494	788.837	415.810	1248.420	-46.578
1500	910.825	1602.319	1016.156	879.245	417.290	1307.850	-45.542
1600	922.737	1661.492	1054.656	970.938	418.886	1367.167	-44.633
1700	933.050	1717.750	1092.021	1063.739	420.533	1426.359	-43.826
1800	942.025	1771.341	1128.284	1157.503	422.163	1485.518	-43.108
1900	949.875	1822.489	1163.485	1252.107	423.751	1544.535	-42.461
2000	956.771	1871.390	1197.667	1347.447	425.248	1603.496	-41.878
2100	962.856	1918.221	1230.872	1443.434	426.582	1662.372	-41.348
2200	968.248	1963.140	1263.143	1539.995	427.754	1721.190	-40.865
2300	973.045	2006.289	1294.522	1637.064	428.762	1779.960	-40.423
2400	977.329	2047.793	1325.049	1734.587	429.538	1838.639	-40.016
2500	981.168	2087.769	1354.763	1832.515	430.096	1897.406	-39.643
2600	984.620	2126.320	1383.701	1930.807	430.402	1956.037	-39.296
2700	987.734	2163.539	1411.899	2029.428	430.463	2014.737	-38.977
2800	990.552	2199.512	1439.389	2128.344	430.252	2073.457	-38.680
2900	993.109	2234.317	1466.204	2227.529	429.743	2132.138	-38.403
3000	995.436	2268.025	1492.372	2326.958	428.981	2190.869	-38.146
3100	997.559	2300.700	1517.923	2426.610	427.889	2249.550	-37.904
3200	999.501	2332.403	1542.883	2526.464	426.509	2308.347	-37.679
3300	1001.281	2363.187	1567.276	2626.505	424.826	2367.233	-37.469
3400	1002.917	2393.102	1591.127	2726.716	422.809	2426.084	-37.271
3500	1004.424	2422.197	1614.458	2827.084	420.466	2484.981	-37.086
3600	1005.814	2450.512	1637.291	2927.597	417.819	2544.041	-36.912
3700	1007.099	2478.088	1659.644	3028.243	414.838	2603.193	-36.750
3800	1008.290	2504.961	1681.537	3129.013	411.497	2662.372	-36.596
3900	1009.395	2531.167	1702.988	3229.898	407.837	2721.587	-36.451
4000	1010.422	2556.735	1724.013	3330.890	403.843	2781.045	-36.316
4100	1011.379	2581.697	1744.629	3431.980	399.478	2840.531	-36.188
4200	1012.271	2606.080	1764.851	3533.163	394.772	2900.119	-36.068
4300	1013.104	2629.909	1784.692	3634.433	389.711	2959.731	-35.953
4400	1013.883	2653.209	1804.167	3735.782	384.304	3019.557	-35.846
4500	1014.613	2676.002	1823.289	3837.207	378.566	3079.566	-35.746
4600	1015.298	2698.310	1842.070	3938.703	372.444	3139.719	-35.652
4700	1015.941	2720.152	1860.521	4040.266	365.954	3199.891	-35.562
4800	1016.545	2741.547	1878.653	4141.890	359.142	3260.314	-35.479
4900	1017.114	2762.514	1896.478	4243.574	351.933	3320.743	-35.399
5000	1017.651	2783.067	1914.005	4345.312	344.423	3381.511	-35.326

3.326. Fluoreno[9,1-*ab*]triphenylene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 136276-45-4
Point Group: C₁

Length: 13.81 Å
Width: 11.09 Å
Breadth: 5.594 Å
L/B Ratio: 1.246

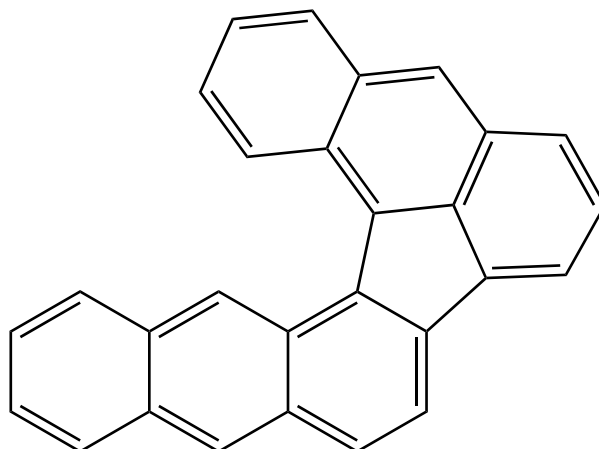
Cartesian coordinates:

C	4.5301	-0.0051	-0.5553	C	-4.5965	-0.9479	-0.3903	H	-5.5461	-0.4100	-0.3055
C	3.1684	-0.0215	-0.2159	C	-4.5652	-2.3002	-0.7471	H	-0.5157	-2.4199	1.2079
C	2.4671	1.1903	-0.1043	C	-3.3565	-2.9630	-0.8977	H	-4.9916	2.1831	0.2548
C	3.1661	2.3946	-0.2899	C	0.3585	2.4010	0.2667	H	-3.8642	4.3666	0.6200
C	4.5116	2.3972	-0.6111	C	-1.0524	2.4439	0.3329	H	-1.3961	4.5693	0.6525
C	5.1960	1.1900	-0.7567	C	-1.7055	1.2297	0.1581	H	0.9246	3.3449	0.2920
C	1.0238	1.1926	0.1353	C	-1.8745	3.5953	0.5046	H	4.2986	-2.4555	-0.0240
C	0.3231	-0.0685	0.1490	C	-3.2414	3.4760	0.4822	H	3.2011	-4.5452	0.7754
C	1.1102	-1.2807	0.3459	C	-3.8983	2.2291	0.2777	H	0.8065	-4.4965	1.4604
C	2.4928	-1.2748	0.0913	C	-3.1305	1.1123	0.1091	H	-1.1955	-2.8529	-0.8187
C	0.5338	-2.4408	0.8853	C	1.2755	-3.5989	1.0445	H	2.6274	3.3484	-0.1831
C	-2.1383	-2.3148	-0.6632	C	2.6214	-3.6216	0.6793	H	5.0393	3.3455	-0.7560
C	-2.1474	-0.9931	-0.2566	C	3.2262	-2.4637	0.2246	H	6.2578	1.1909	-1.0232
C	-1.0558	-0.0346	0.0185	H	-3.3489	-4.0131	-1.2086	H	5.0645	-0.9632	-0.6464
C	-3.3984	-0.3013	-0.1644	H	-5.5055	-2.8324	-0.9241				

Table 3.326: Table of thermodynamic data as a function of temperature for Fluoreno[9,1-*ab*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-52.334	524.931	524.931	∞
100	116.047	358.006	810.208	-45.220	551.202	598.649	-312.696
200	225.992	470.361	612.281	-28.384	537.359	651.605	-170.178
250	290.207	527.629	589.598	-15.492	530.794	680.925	-142.269
298.15	353.189	584.138	584.138	0.000	524.931	710.386	-124.454
300	355.585	586.330	584.145	0.656	524.714	711.536	-123.887
350	418.676	645.928	588.707	20.027	519.306	743.113	-110.901
400	477.291	705.718	599.598	42.448	514.615	775.404	-101.255
450	530.429	765.059	614.693	67.665	510.559	808.251	-93.817
500	577.935	823.452	632.659	95.397	507.051	841.541	-87.913
600	657.571	936.151	673.933	157.331	501.369	909.003	-79.134
700	720.499	1042.427	719.063	226.355	497.245	977.295	-72.925
800	770.926	1142.047	765.778	301.015	494.494	1046.066	-68.300
900	811.995	1235.300	812.824	380.229	492.935	1115.102	-64.717
1000	845.907	1322.663	859.486	463.176	492.407	1184.268	-61.859
1100	874.217	1404.653	905.359	549.224	492.711	1253.456	-59.520
1200	898.059	1481.771	950.212	637.871	493.706	1322.566	-57.569
1300	918.284	1554.475	993.924	728.715	495.210	1391.582	-55.913
1400	935.550	1623.175	1036.440	821.429	497.092	1460.472	-54.490
1500	950.377	1688.240	1077.744	915.744	499.271	1529.219	-53.251
1600	963.177	1749.994	1117.846	1011.437	501.616	1597.804	-52.162
1700	974.284	1808.728	1156.773	1108.323	504.054	1666.215	-51.195
1800	983.968	1864.697	1194.560	1206.247	506.509	1734.547	-50.334
1900	992.451	1918.129	1231.247	1305.077	508.951	1802.689	-49.558
2000	999.916	1969.229	1266.878	1404.703	511.326	1870.731	-48.857
2100	1006.510	2018.178	1301.497	1505.031	513.554	1938.643	-48.220
2200	1012.361	2065.139	1335.148	1605.980	515.635	2006.455	-47.638
2300	1017.571	2110.257	1367.874	1707.482	517.564	2074.174	-47.105
2400	1022.227	2153.665	1399.716	1809.476	519.271	2141.765	-46.613
2500	1026.403	2195.480	1430.716	1911.911	520.766	2209.405	-46.162
2600	1030.161	2235.811	1460.910	2014.743	522.013	2276.870	-45.742
2700	1033.553	2274.754	1490.335	2117.931	523.018	2344.367	-45.354
2800	1036.624	2312.399	1519.026	2221.443	523.753	2411.853	-44.993
2900	1039.413	2348.824	1547.015	2325.247	524.189	2479.264	-44.655
3000	1041.951	2384.106	1574.333	2429.317	524.371	2546.691	-44.341
3100	1044.268	2418.309	1601.010	2533.630	524.220	2614.038	-44.045
3200	1046.388	2451.498	1627.071	2638.164	523.779	2681.470	-43.770
3300	1048.333	2483.727	1652.545	2742.901	523.028	2748.961	-43.512
3400	1050.120	2515.050	1677.454	2847.825	521.940	2816.391	-43.268
3500	1051.767	2545.514	1701.822	2952.921	520.519	2883.838	-43.038
3600	1053.287	2575.165	1725.672	3058.174	518.789	2951.421	-42.823
3700	1054.692	2604.043	1749.023	3163.574	516.717	3019.074	-42.621
3800	1055.994	2632.188	1771.896	3269.109	514.276	3086.726	-42.429
3900	1057.203	2659.633	1794.308	3374.770	511.509	3154.393	-42.247
4000	1058.327	2686.414	1816.277	3480.547	508.398	3222.279	-42.078
4100	1059.374	2712.560	1837.820	3586.433	504.908	3290.170	-41.916
4200	1060.350	2738.100	1858.952	3692.420	501.066	3358.143	-41.764
4300	1061.262	2763.061	1879.689	3798.501	496.859	3426.118	-41.618
4400	1062.116	2787.469	1900.044	3904.670	492.297	3494.290	-41.482
4500	1062.915	2811.347	1920.031	4010.922	487.393	3562.626	-41.353
4600	1063.665	2834.717	1939.662	4117.252	482.094	3631.085	-41.231
4700	1064.369	2857.600	1958.950	4223.654	476.416	3699.546	-41.115
4800	1065.031	2880.015	1977.906	4330.124	470.406	3768.240	-41.006
4900	1065.655	2901.982	1996.542	4436.659	463.989	3836.924	-40.901
5000	1066.243	2923.517	2014.866	4543.254	457.260	3905.935	-40.804

3.327. Anthra[1,2-*a*]aceanthrylene



Formula: $C_{28}H_{16}$
Mass: 352.427 g/mol
CAS Number: 203-06-5
Point Group: C_1

Length: 15.25 Å
Width: 11.87 Å
Breadth: 4.971 Å
L/B Ratio: 1.284

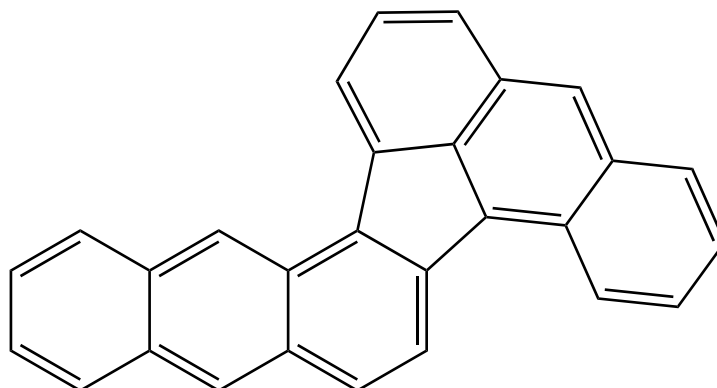
Cartesian coordinates:

C	-0.2378	0.8460	-0.1078	C	-3.2770	2.9206	0.1396	H	6.0246	1.4824	-0.3204
C	-0.8046	2.1286	-0.1472	C	-4.5987	2.4133	0.3440	H	3.3742	-2.5939	0.8490
C	5.3225	-1.7463	0.5756	C	-4.8681	1.0755	0.4177	H	3.9333	2.7674	-0.5263
C	6.0786	-0.5853	0.2393	C	-1.3410	-0.1434	-0.0387	H	1.3067	-1.3394	0.5353
C	5.4530	0.5835	-0.0633	C	-2.5216	0.6220	0.1175	H	1.9310	4.0701	-0.6562
C	3.9634	-1.7063	0.5919	C	-3.8134	0.1143	0.2871	H	-0.5522	4.2677	-0.4059
C	3.2678	-0.4950	0.2685	C	-3.9407	-1.2771	0.2955	H	-3.1127	4.0008	0.0720
C	4.0222	0.6649	-0.0506	C	-1.5089	-1.5304	-0.1671	H	-5.4138	3.1391	0.4394
C	3.3538	1.8592	-0.3178	C	-2.8170	-2.0790	0.0549	H	-5.8904	0.7129	0.5708
C	1.8735	-0.4389	0.2595	C	-2.9918	-3.5027	-0.0006	H	-4.9214	-1.7375	0.4648
C	1.1896	0.7349	-0.0683	C	-1.9634	-4.3245	-0.3366	H	-3.9832	-3.9125	0.2263
C	1.9560	1.9203	-0.3009	C	-0.6909	-3.7745	-0.6563	H	-2.0985	-5.4101	-0.3796
C	1.3099	3.1879	-0.4631	C	-0.4765	-2.4341	-0.5731	H	0.1094	-4.4491	-0.9783
C	-0.0422	3.3009	-0.3421	H	5.8590	-2.6691	0.8192	H	0.5028	-2.0180	-0.8459
C	-2.2525	2.0308	0.0342	H	7.1713	-0.6548	0.2320				

Table 3.327: Table of thermodynamic data as a function of temperature for Anthra[1,2-*a*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-52.182	550.460	550.460	∞
100	114.193	356.100	808.085	-45.199	576.754	624.391	-326.142
200	226.088	467.756	610.014	-28.452	562.820	677.588	-176.964
250	290.962	525.123	587.271	-15.537	556.279	707.036	-147.724
298.15	354.240	581.795	581.795	0.000	550.460	736.615	-129.049
300	356.642	583.993	581.801	0.658	550.246	737.768	-128.454
350	419.798	643.761	586.377	20.084	544.892	769.458	-114.833
400	478.357	703.699	597.298	42.560	540.256	801.854	-104.709
450	531.396	763.159	612.431	67.828	536.252	834.798	-96.899
500	578.797	821.649	630.438	95.605	532.790	868.181	-90.696
600	658.263	934.489	671.794	157.617	527.185	935.816	-81.468
700	721.087	1040.863	717.000	226.704	523.124	1004.269	-74.938
800	771.454	1140.557	763.782	301.420	520.428	1073.192	-70.071
900	812.486	1233.870	810.887	380.685	518.921	1142.374	-66.300
1000	846.371	1321.283	857.603	463.680	518.440	1211.681	-63.290
1100	874.657	1403.317	903.523	549.773	518.789	1281.004	-60.829
1200	898.477	1480.472	948.420	638.463	519.827	1350.246	-58.773
1300	918.679	1553.208	992.172	729.348	521.372	1419.391	-57.031
1400	935.924	1621.937	1034.723	822.100	523.292	1488.406	-55.532
1500	950.728	1687.027	1076.059	916.451	525.507	1557.275	-54.228
1600	963.507	1748.803	1116.192	1012.178	527.886	1625.980	-53.082
1700	974.594	1807.556	1155.147	1109.096	530.356	1694.509	-52.065
1800	984.259	1863.542	1192.959	1207.050	532.842	1762.958	-51.159
1900	992.724	1916.990	1229.670	1305.908	535.312	1831.215	-50.343
2000	1000.171	1968.103	1265.323	1405.561	537.713	1899.370	-49.605
2100	1006.750	2017.064	1299.963	1505.913	539.965	1967.393	-48.935
2200	1012.585	2064.036	1333.633	1606.886	542.070	2035.316	-48.324
2300	1017.782	2109.164	1366.377	1708.409	544.021	2103.146	-47.763
2400	1022.425	2152.580	1398.237	1810.424	545.748	2170.845	-47.246
2500	1026.590	2194.403	1429.252	1912.878	547.262	2238.594	-46.772
2600	1030.337	2234.741	1459.461	2015.728	548.528	2306.166	-46.330
2700	1033.719	2273.691	1488.901	2118.933	549.549	2373.769	-45.922
2800	1036.780	2311.341	1517.605	2222.461	550.301	2441.361	-45.543
2900	1039.560	2347.772	1545.607	2326.280	550.752	2508.877	-45.189
3000	1042.091	2383.058	1572.937	2430.364	550.949	2576.409	-44.858
3100	1044.400	2417.267	1599.624	2534.691	550.811	2643.861	-44.548
3200	1046.514	2450.459	1625.697	2639.238	550.382	2711.397	-44.258
3300	1048.452	2482.692	1651.181	2743.988	549.644	2778.992	-43.987
3400	1050.233	2514.018	1676.100	2848.923	548.567	2846.525	-43.731
3500	1051.874	2544.486	1700.477	2954.030	547.158	2914.075	-43.489
3600	1053.389	2574.140	1724.336	3059.294	545.438	2981.761	-43.263
3700	1054.790	2603.021	1747.695	3164.704	543.376	3049.516	-43.051
3800	1056.087	2631.168	1770.576	3270.248	540.944	3117.270	-42.849
3900	1057.292	2658.616	1792.996	3375.918	538.186	3185.039	-42.658
4000	1058.412	2685.398	1814.972	3481.704	535.084	3253.027	-42.479
4100	1059.455	2711.546	1836.522	3587.598	531.602	3321.020	-42.309
4200	1060.428	2737.088	1857.662	3693.593	527.769	3389.093	-42.149
4300	1061.337	2762.051	1878.405	3799.681	523.569	3457.169	-41.995
4400	1062.187	2786.461	1898.766	3905.858	519.014	3525.442	-41.851
4500	1062.983	2810.340	1918.759	4012.117	514.117	3593.879	-41.716
4600	1063.730	2833.712	1938.396	4118.453	508.825	3662.439	-41.587
4700	1064.432	2856.596	1957.690	4224.861	503.154	3731.000	-41.465
4800	1065.092	2879.013	1976.651	4331.338	497.150	3799.794	-41.349
4900	1065.713	2900.981	1995.291	4437.879	490.739	3868.578	-41.239
5000	1066.299	2922.517	2013.621	4544.479	484.016	3937.689	-41.136

3.328. Anthra[2,1-*a*]aceanthrylene



Formula: $C_{28}H_{16}$
Mass: 352.427 g/mol
CAS Number: 203-21-4
Point Group: C_s

Length: 17.24 Å
Width: 10.81 Å
Breadth: 3.889 Å
L/B Ratio: 1.595

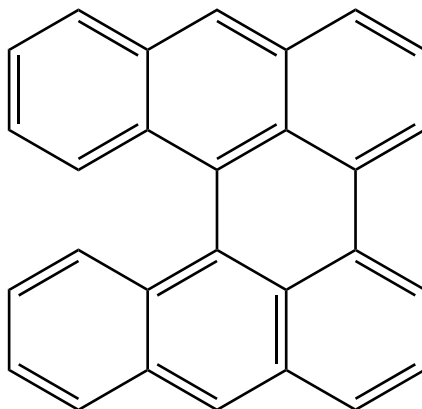
Cartesian coordinates:

C	-5.7987	-1.2082	0.0000	C	1.8202	1.0559	-0.0000	H	6.5542	0.3456	0.0000
C	-4.4017	-0.8850	0.0000	C	2.8485	2.0026	-0.0000	H	2.7813	-2.9405	0.0000
C	-4.0130	0.4835	0.0000	C	4.1565	1.5040	-0.0000	H	5.0053	2.1982	-0.0000
C	-5.0310	1.4934	0.0000	C	4.3861	0.1191	-0.0000	H	3.2018	4.1555	0.0000
C	-6.3459	1.1484	0.0000	C	3.3151	-0.8322	-0.0000	H	0.8000	4.7476	0.0000
C	-6.7356	-0.2233	0.0000	C	2.4334	3.3749	-0.0000	H	-0.9899	3.0112	0.0000
C	-2.6593	0.8178	0.0000	C	1.1041	3.6950	0.0000	H	-1.4013	-3.6259	-0.0000
C	-1.6797	-0.1809	-0.0000	C	0.0672	2.7083	0.0000	H	1.0387	-3.0623	-0.0000
C	-2.0663	-1.5541	-0.0000	C	0.4201	1.3934	-0.0000	H	-2.3487	1.8755	0.0000
C	-3.4265	-1.8828	0.0000	C	5.7315	-0.3789	0.0000	H	-3.7298	-2.9373	-0.0000
C	-0.2865	0.1056	-0.0000	C	5.9836	-1.7153	0.0000	H	-4.7217	2.5446	0.0000
C	0.6614	-0.9255	-0.0000	C	4.9135	-2.6554	0.0000	H	-7.1270	1.9156	0.0000
C	0.2637	-2.2821	-0.0000	C	3.6219	-2.2293	0.0000	H	-7.8035	-0.4651	-0.0000
C	-1.0678	-2.5817	-0.0000	H	5.1512	-3.7242	0.0000	H	-6.0890	-2.2650	-0.0000
C	2.0090	-0.3404	-0.0000	H	7.0123	-2.0906	0.0000				

Table 3.328: Table of thermodynamic data as a function of temperature for Anthra[2,1-*a*]aceanthrylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-52.635	530.515	530.515	∞
100	116.034	362.974	817.318	-45.434	556.572	603.522	-315.241
200	227.213	475.615	618.362	-28.549	542.777	655.973	-171.319
250	291.956	533.219	595.546	-15.582	536.289	685.022	-143.125
298.15	355.111	590.055	590.055	0.000	530.515	714.206	-125.123
300	357.508	592.259	590.062	0.659	530.302	715.344	-124.550
350	420.535	652.151	594.648	20.126	524.989	746.617	-111.424
400	478.973	712.178	605.589	42.636	520.386	778.592	-101.672
450	531.903	771.705	620.747	67.931	516.410	811.111	-94.149
500	579.211	830.243	638.779	95.732	512.970	844.065	-88.177
600	658.532	943.145	680.183	157.777	507.399	910.836	-79.294
700	721.249	1049.552	725.430	226.885	503.360	978.422	-73.009
800	771.540	1149.263	772.246	301.614	500.676	1046.475	-68.326
900	812.517	1242.583	819.378	380.884	499.174	1114.787	-64.699
1000	846.363	1329.997	866.116	463.880	498.695	1183.222	-61.804
1100	874.624	1412.028	912.055	549.971	499.041	1251.674	-59.436
1200	898.425	1489.180	956.966	638.657	500.075	1320.045	-57.459
1300	918.617	1561.911	1000.730	729.536	501.614	1388.319	-55.782
1400	935.855	1630.636	1043.292	822.282	503.528	1456.464	-54.340
1500	950.656	1695.720	1084.637	916.626	505.736	1524.464	-53.085
1600	963.434	1757.492	1124.776	1012.346	508.108	1592.300	-51.982
1700	974.521	1816.240	1163.737	1109.256	510.571	1659.960	-51.003
1800	984.187	1872.222	1201.554	1207.202	513.049	1727.541	-50.131
1900	992.654	1925.666	1238.270	1306.054	515.512	1794.930	-49.345
2000	1000.104	1976.776	1273.927	1405.699	517.906	1862.217	-48.635
2100	1006.685	2025.734	1308.570	1506.046	520.152	1929.374	-47.990
2200	1012.524	2072.703	1342.243	1607.012	522.250	1996.429	-47.400
2300	1017.723	2117.828	1374.989	1708.529	524.196	2063.393	-46.860
2400	1022.369	2161.242	1406.851	1810.538	525.916	2130.226	-46.362
2500	1026.536	2203.063	1437.868	1912.987	527.425	2197.108	-45.905
2600	1030.286	2243.399	1468.079	2015.831	528.686	2263.815	-45.480
2700	1033.670	2282.347	1497.520	2119.032	529.702	2330.552	-45.086
2800	1036.734	2319.995	1526.226	2222.555	530.449	2397.279	-44.721
2900	1039.516	2356.425	1554.228	2326.369	530.896	2463.929	-44.379
3000	1042.049	2391.709	1581.559	2430.450	531.088	2530.596	-44.061
3100	1044.361	2425.916	1608.248	2534.772	530.946	2597.183	-43.761
3200	1046.476	2459.107	1634.321	2639.315	530.514	2663.854	-43.482
3300	1048.416	2491.339	1659.805	2744.061	529.772	2730.584	-43.221
3400	1050.199	2522.664	1684.725	2848.993	528.692	2797.252	-42.974
3500	1051.841	2553.131	1709.103	2954.096	527.279	2863.939	-42.741
3600	1053.357	2582.784	1732.962	3059.357	525.556	2930.760	-42.523
3700	1054.760	2611.664	1756.322	3164.764	523.490	2997.651	-42.318
3800	1056.059	2639.810	1779.203	3270.306	521.056	3064.540	-42.124
3900	1057.264	2667.257	1801.624	3375.972	518.295	3131.445	-41.940
4000	1058.386	2694.039	1823.600	3481.756	515.190	3198.569	-41.768
4100	1059.430	2720.187	1845.151	3587.647	511.706	3265.697	-41.605
4200	1060.404	2745.728	1866.290	3693.639	507.870	3332.907	-41.450
4300	1061.313	2770.691	1887.034	3799.726	503.668	3400.119	-41.302
4400	1062.165	2795.100	1907.395	3905.900	499.111	3467.528	-41.164
4500	1062.962	2818.979	1927.388	4012.157	494.211	3535.101	-41.034
4600	1063.710	2842.350	1947.026	4118.491	488.917	3602.797	-40.910
4700	1064.412	2865.234	1966.319	4224.897	483.244	3670.494	-40.792
4800	1065.073	2887.650	1985.281	4331.372	477.238	3738.425	-40.682
4900	1065.695	2909.618	2003.922	4437.910	470.825	3806.345	-40.575
5000	1066.281	2931.153	2022.252	4544.510	464.100	3874.593	-40.477

3.329. Dibenzo[*a,o*]perylene



Other names: o-meso-Benzodianthrene

Formula: C₂₈H₁₆

Mass: 352.427 g/mol

CAS Number: 190-36-3

Point Group: C₂

Length: 11.96 Å

Width: 11.32 Å

Breadth: 6.634 Å

L/B Ratio: 1.056

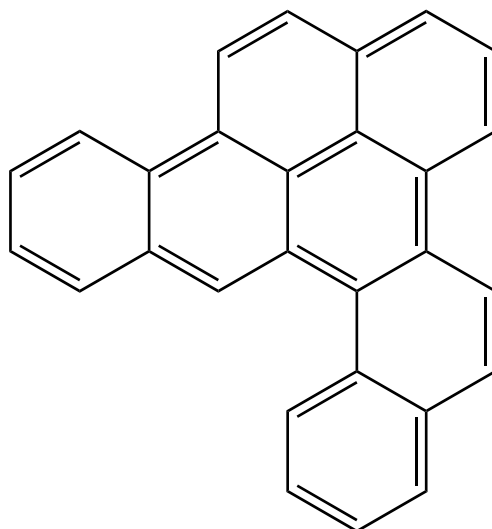
Cartesian coordinates:

C	3.7062	-2.3342	0.4634	C	-2.9203	-1.1749	-0.1508	H	-0.0872	-2.3290	1.3422
C	2.9192	-1.1775	0.1519	C	-3.5309	-0.0272	0.3595	H	-4.7764	-2.3137	-0.2157
C	1.5161	-1.1998	0.3907	C	-2.7927	1.1484	0.5043	H	-4.6014	-0.0348	0.5991
C	0.9769	-2.3395	1.0719	C	-0.9797	-2.3385	-1.0723	H	-0.8051	4.5070	0.4690
C	1.7603	-3.4020	1.4029	C	-1.7645	-3.3998	-1.4037	H	-3.1958	4.4836	1.1800
C	3.1426	-3.4147	1.0663	C	-3.1467	-3.4113	-1.0664	H	-4.4910	2.3583	1.1343
C	0.7319	-0.0818	0.0244	C	-3.7086	-2.3305	-0.4624	H	4.4938	2.3536	-1.1338
C	1.3968	1.1320	-0.2507	C	-1.3483	3.5515	0.5289	H	3.2005	4.4803	-1.1803
C	2.7942	1.1456	-0.5041	C	-2.7178	3.5397	0.8982	H	0.8100	4.5062	-0.4684
C	3.5314	-0.0304	-0.3578	C	-3.4255	2.3764	0.8787	H	4.6020	-0.0393	-0.5964
C	-0.7320	-0.0809	-0.0254	C	3.4282	2.3728	-0.8788	H	0.0844	-2.3294	-1.3427
C	-1.3955	1.1335	0.2500	C	2.7216	3.5369	-0.8987	H	1.3392	-4.2599	1.9371
C	-0.6952	2.3864	0.2159	C	1.3522	3.5502	-0.5290	H	3.7402	-4.2980	1.3134
C	0.6979	2.3857	-0.2162	H	-3.7453	-4.2938	-1.3137	H	4.7741	-2.3183	0.2174
C	-1.5174	-1.1983	-0.3908	H	-1.3450	-4.2574	-1.9398				

Table 3.329: Table of thermodynamic data as a function of temperature for Dibenzo[*a,o*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-51.820	542.862	542.862	∞
100	112.046	342.658	793.431	-45.077	569.277	618.258	-322.938
200	225.710	453.461	595.675	-28.443	555.231	672.858	-175.729
250	290.901	510.782	572.935	-15.538	548.680	703.023	-146.885
298.15	354.346	567.458	567.458	0.000	542.862	733.291	-128.467
300	356.753	569.657	567.465	0.658	542.648	734.471	-127.880
350	420.028	629.452	572.043	20.093	537.304	766.877	-114.448
400	478.676	689.426	582.969	42.583	532.681	799.988	-104.466
450	531.779	748.928	598.110	67.868	528.694	833.645	-96.765
500	579.219	807.460	616.128	95.666	525.252	867.738	-90.650
600	658.706	920.380	657.511	157.721	519.691	936.788	-81.553
700	721.500	1026.820	702.747	226.851	515.674	1006.648	-75.115
800	771.817	1126.567	749.559	301.606	513.017	1076.973	-70.318
900	812.795	1219.919	796.692	380.904	511.543	1147.552	-66.601
1000	846.629	1307.362	843.434	463.928	511.090	1218.252	-63.634
1100	874.872	1389.418	889.378	550.044	511.463	1288.967	-61.207
1200	898.655	1466.591	934.296	638.754	512.520	1359.597	-59.180
1300	918.827	1539.340	978.067	729.655	514.081	1430.129	-57.462
1400	936.047	1608.079	1020.635	822.421	516.015	1500.531	-55.984
1500	950.832	1673.176	1061.987	916.784	518.242	1570.785	-54.698
1600	963.595	1734.959	1102.134	1012.520	520.631	1640.875	-53.568
1700	974.668	1793.717	1141.101	1109.446	523.109	1710.789	-52.565
1800	984.323	1849.707	1178.925	1207.407	525.601	1780.621	-51.671
1900	992.779	1903.158	1215.647	1306.271	528.077	1850.261	-50.866
2000	1000.219	1954.274	1251.309	1405.929	530.483	1919.799	-50.139
2100	1006.791	2003.237	1285.958	1506.286	532.740	1989.206	-49.478
2200	1012.622	2050.210	1319.636	1607.262	534.848	2058.511	-48.874
2300	1017.814	2095.340	1352.388	1708.789	536.803	2127.723	-48.321
2400	1022.454	2138.757	1384.254	1810.806	538.533	2196.805	-47.811
2500	1026.615	2180.582	1415.276	1913.264	540.050	2265.936	-47.343
2600	1030.359	2220.920	1445.491	2016.116	541.318	2334.890	-46.908
2700	1033.739	2259.871	1474.936	2119.323	542.342	2403.876	-46.505
2800	1036.799	2297.522	1503.646	2222.853	543.095	2472.850	-46.131
2900	1039.577	2333.954	1531.652	2326.674	543.548	2541.747	-45.781
3000	1042.106	2369.240	1558.987	2430.760	543.746	2610.661	-45.455
3100	1044.414	2403.449	1585.679	2535.088	543.610	2679.494	-45.148
3200	1046.527	2436.642	1611.755	2639.636	543.182	2748.413	-44.862
3300	1048.464	2468.875	1637.243	2744.387	542.445	2817.389	-44.595
3400	1050.244	2500.202	1662.165	2849.324	541.370	2886.304	-44.342
3500	1051.884	2530.670	1686.546	2954.431	539.962	2955.236	-44.104
3600	1053.398	2560.324	1710.408	3059.696	538.243	3024.303	-43.881
3700	1054.798	2589.205	1733.771	3165.107	536.181	3093.440	-43.671
3800	1056.095	2617.352	1756.654	3270.653	533.751	3162.576	-43.472
3900	1057.300	2644.800	1779.077	3376.323	530.993	3231.726	-43.283
4000	1058.419	2671.583	1801.056	3482.110	527.892	3301.095	-43.107
4100	1059.462	2697.731	1822.608	3588.004	524.411	3370.470	-42.939
4200	1060.434	2723.273	1843.750	3694.000	520.578	3439.925	-42.781
4300	1061.343	2748.237	1864.495	3800.089	516.379	3509.382	-42.630
4400	1062.192	2772.646	1884.859	3906.266	511.825	3579.036	-42.488
4500	1062.989	2796.526	1904.854	4012.526	506.928	3648.855	-42.354
4600	1063.735	2819.897	1924.493	4118.862	501.637	3718.796	-42.227
4700	1064.437	2842.782	1943.788	4225.271	495.966	3788.739	-42.106
4800	1065.096	2865.199	1962.751	4331.748	489.963	3858.915	-41.993
4900	1065.717	2887.167	1981.394	4438.289	483.552	3929.080	-41.884
5000	1066.303	2908.703	1999.725	4544.891	476.829	3999.572	-41.782

3.330. Phenanthro[1,2,3,4-*def*]chrysene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 137570-58-2
Point Group: C₁

Length: 13.96 Å
Width: 12.54 Å
Breadth: 5.056 Å
L/B Ratio: 1.113

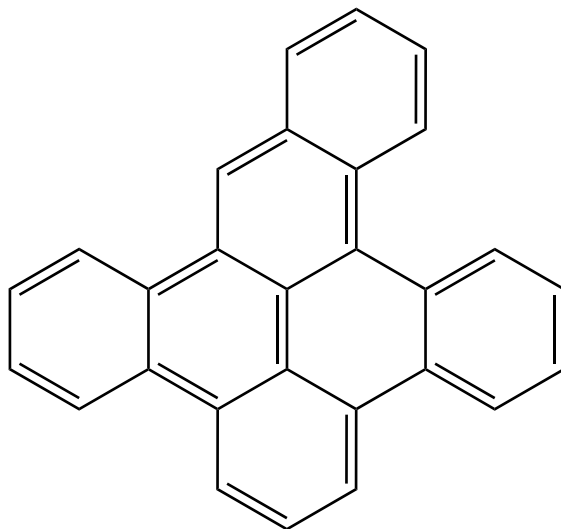
Cartesian coordinates:

C	-3.4425	3.8855	-0.4137	C	-2.4115	-0.1819	0.1676	H	-4.9015	0.8861	0.3454
C	-4.4492	2.9469	-0.0991	C	-3.4137	-1.1803	0.3905	H	-1.3465	4.2128	-0.7475
C	-4.1274	1.6311	0.1063	C	-3.0951	-2.4978	0.4403	H	0.3316	2.4999	-0.5580
C	-2.1339	3.4899	-0.5052	C	1.3666	-0.0009	-0.0750	H	-2.2027	-5.0381	0.3469
C	-1.7775	2.1330	-0.2844	C	1.6509	-1.3529	-0.2524	H	0.1442	-5.7436	-0.0786
C	-2.7817	1.1931	0.0099	C	2.9847	-1.7785	-0.5093	H	1.9232	-4.0541	-0.4008
C	-0.4172	1.7259	-0.3341	C	4.0171	-0.8922	-0.5187	H	-4.4538	-0.8403	0.5127
C	-0.0352	0.4270	-0.0938	C	2.4713	0.9071	0.1108	H	-3.8639	-3.2597	0.6119
C	0.6054	-2.3647	-0.1492	C	3.7850	0.4637	-0.1601	H	3.1655	-2.8448	-0.7138
C	-1.4143	-4.2909	0.2027	C	4.8867	1.3496	-0.0323	H	5.0359	-1.2140	-0.7629
C	-0.1131	-4.6801	-0.0325	C	4.7017	2.6279	0.4203	H	5.8882	0.9874	-0.2915
C	0.8907	-3.7232	-0.2125	C	3.4074	3.0573	0.7789	H	5.5466	3.3164	0.5218
C	-1.7417	-2.9222	0.2471	C	2.3307	2.2237	0.6284	H	3.2725	4.0648	1.1863
C	-0.7322	-1.9526	0.0742	H	-3.7206	4.9310	-0.5816	H	1.3357	2.5806	0.9278
C	-1.0677	-0.5601	0.0706	H	-5.4886	3.2827	-0.0239				

Table 3.330: Table of thermodynamic data as a function of temperature for Phenanthro[1,2,3,4-*def*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.732	468.468	468.468	∞
100	112.529	355.214	803.270	-44.806	495.154	542.880	-283.565
200	224.108	465.569	606.809	-28.248	481.032	596.236	-155.718
250	288.880	522.483	584.223	-15.435	474.389	625.806	-130.752
298.15	352.087	578.782	578.782	0.000	468.468	655.521	-114.842
300	354.488	580.967	578.788	0.654	468.249	656.680	-114.336
350	417.650	640.402	583.338	19.973	462.788	688.529	-102.755
400	476.282	700.057	594.201	42.342	458.046	721.100	-94.164
450	529.435	759.279	609.259	67.509	453.941	754.233	-87.547
500	576.967	817.569	627.185	95.192	450.384	787.815	-82.301
600	656.688	930.098	668.376	157.033	444.609	855.874	-74.509
700	719.722	1036.246	713.426	225.974	440.402	924.778	-69.006
800	770.255	1135.770	760.067	300.562	437.578	994.172	-64.911
900	811.418	1228.949	807.045	379.714	435.957	1063.840	-61.742
1000	845.410	1316.255	853.648	462.607	435.375	1133.644	-59.214
1100	873.788	1398.202	899.466	548.609	435.632	1203.475	-57.147
1200	897.686	1475.285	944.271	637.216	436.588	1273.231	-55.421
1300	917.957	1547.960	987.941	728.025	438.057	1342.898	-53.957
1400	935.263	1616.638	1030.418	820.709	439.908	1412.441	-52.698
1500	950.123	1681.684	1071.686	914.997	442.060	1481.842	-51.601
1600	962.951	1743.423	1111.757	1010.666	444.381	1551.084	-50.637
1700	974.081	1802.143	1150.655	1107.530	446.798	1620.152	-49.780
1800	983.786	1858.101	1188.415	1205.434	449.234	1689.144	-49.017
1900	992.287	1911.525	1225.079	1304.247	451.659	1757.946	-48.328
2000	999.766	1962.616	1260.688	1403.858	454.017	1826.649	-47.706
2100	1006.374	2011.558	1295.286	1504.172	456.231	1895.222	-47.140
2200	1012.236	2058.513	1328.918	1605.108	458.300	1963.696	-46.623
2300	1017.456	2103.626	1361.627	1706.597	460.217	2032.079	-46.149
2400	1022.122	2147.029	1393.454	1808.581	461.912	2100.333	-45.712
2500	1026.306	2188.840	1424.438	1911.006	463.397	2168.637	-45.310
2600	1030.071	2229.167	1454.618	2013.828	464.636	2236.766	-44.936
2700	1033.469	2268.107	1484.030	2117.008	465.631	2304.927	-44.591
2800	1036.546	2305.749	1512.709	2220.511	466.359	2373.078	-44.269
2900	1039.340	2342.172	1540.687	2324.308	466.787	2441.153	-43.969
3000	1041.883	2377.451	1567.994	2428.371	466.962	2509.246	-43.689
3100	1044.204	2411.652	1594.660	2532.677	466.804	2577.258	-43.426
3200	1046.328	2444.839	1620.712	2637.205	466.357	2645.356	-43.180
3300	1048.276	2477.066	1646.176	2741.937	465.600	2713.514	-42.950
3400	1050.067	2508.387	1671.077	2846.855	464.507	2781.609	-42.733
3500	1051.716	2538.850	1695.437	2951.945	463.081	2849.723	-42.529
3600	1053.239	2568.500	1719.279	3057.194	461.346	2917.973	-42.338
3700	1054.647	2597.377	1742.623	3162.589	459.269	2986.292	-42.158
3800	1055.952	2625.520	1765.488	3268.120	456.824	3054.611	-41.988
3900	1057.163	2652.964	1787.894	3373.776	454.052	3122.945	-41.826
4000	1058.288	2679.744	1809.856	3479.550	450.937	3191.498	-41.676
4100	1059.337	2705.889	1831.393	3585.431	447.443	3260.056	-41.533
4200	1060.315	2731.428	1852.520	3691.415	443.598	3328.695	-41.398
4300	1061.229	2756.389	1873.251	3797.492	439.388	3397.338	-41.269
4400	1062.083	2780.796	1893.601	3903.658	434.822	3466.177	-41.148
4500	1062.884	2804.673	1913.582	4009.907	429.915	3535.181	-41.034
4600	1063.635	2828.042	1933.209	4116.234	424.613	3604.307	-40.927
4700	1064.341	2850.925	1952.492	4222.633	418.932	3673.435	-40.825
4800	1065.004	2873.340	1971.444	4329.100	412.920	3742.797	-40.729
4900	1065.629	2895.306	1990.075	4435.632	406.500	3812.148	-40.637
5000	1066.218	2916.840	2008.395	4542.225	399.769	3881.827	-40.552

3.331. Benzo[fg]naphtho[1,2,3-op]naphthacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 137570-59-3
Point Group: C₁

Length: 13.72 Å
Width: 11.88 Å
Breadth: 5.141 Å
L/B Ratio: 1.155

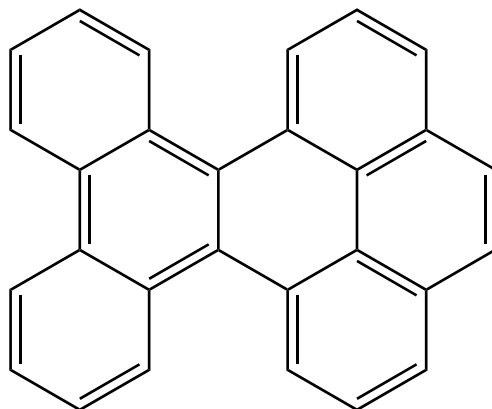
Cartesian coordinates:

C	0.9894	-1.2592	-0.1287	C	4.3975	0.3334	-0.0469	H	2.3004	4.6869	0.8410
C	0.4403	-2.5187	-0.1709	C	-2.0818	0.9217	-0.1980	H	-0.1685	4.4546	0.6163
C	2.1350	1.3433	0.1878	C	-1.5156	2.1947	0.0046	H	2.8406	-3.1817	-0.5298
C	2.6796	2.6005	0.4458	C	-2.3215	3.3452	-0.0936	H	5.3075	-2.8913	-0.6023
C	1.8581	3.7095	0.6226	C	-3.6470	3.2545	-0.4608	H	6.3060	-0.6333	-0.2826
C	0.4864	3.5769	0.5076	C	-4.1902	2.0026	-0.7639	H	4.8314	1.3349	0.0963
C	0.1322	-0.1177	-0.0294	C	-3.4200	0.8648	-0.6370	H	-1.8698	4.3268	0.1165
C	0.7309	1.1898	0.1136	C	-0.9498	-2.7079	0.0056	H	-4.2662	4.1541	-0.5340
C	-0.0895	2.3276	0.2343	C	-1.8058	-1.5912	0.1298	H	-5.2278	1.9278	-1.1057
C	-1.2596	-0.2716	-0.0313	C	-3.1591	-1.8519	0.4838	H	-3.8681	-0.1057	-0.8904
C	3.0014	0.1889	-0.0129	C	-3.6354	-3.1287	0.6131	H	-3.8378	-1.0082	0.6689
C	2.4377	-1.0844	-0.1848	C	-2.7874	-4.2363	0.3962	H	-4.6798	-3.3033	0.8924
C	3.2856	-2.1838	-0.3963	C	-1.4676	-4.0287	0.1061	H	-3.1929	-5.2498	0.4772
C	4.6591	-2.0253	-0.4343	H	1.0905	-3.3990	-0.3004	H	-0.7869	-4.8750	-0.0417
C	5.2189	-0.7595	-0.2561	H	3.7732	2.7095	0.5075				

Table 3.331: Table of thermodynamic data as a function of temperature for Benzo[fg]naphtho[1,2,3-*op*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.705	471.127	471.127	∞
100	113.211	353.536	801.550	-44.801	497.817	545.711	-285.044
200	224.064	464.272	605.238	-28.193	483.746	599.210	-156.494
250	288.275	521.112	582.701	-15.397	477.085	628.846	-131.387
298.15	351.172	577.274	577.274	0.000	471.127	658.629	-115.387
300	353.565	579.453	577.280	0.652	470.907	659.791	-114.877
350	416.603	638.735	581.818	19.921	465.396	691.720	-103.231
400	475.226	698.248	592.653	42.238	460.601	724.378	-94.592
450	528.426	757.349	607.676	67.353	456.443	757.605	-87.939
500	576.028	815.536	625.562	94.987	452.838	791.286	-82.663
600	655.891	927.906	666.671	156.742	446.976	859.556	-74.829
700	719.041	1033.940	711.643	225.609	442.695	928.685	-69.298
800	769.660	1133.379	758.213	300.133	439.808	998.314	-65.182
900	810.888	1226.492	805.127	379.229	438.131	1068.225	-61.997
1000	844.932	1313.745	851.673	462.072	437.499	1138.278	-59.456
1100	873.354	1395.648	897.441	548.028	437.711	1208.362	-57.379
1200	897.289	1472.695	942.201	636.594	438.624	1278.375	-55.645
1300	917.594	1545.341	985.829	727.365	440.056	1348.303	-54.174
1400	934.929	1613.993	1028.269	820.013	441.872	1418.108	-52.909
1500	949.815	1679.016	1069.504	914.269	443.992	1487.775	-51.808
1600	962.667	1740.736	1109.543	1009.909	446.284	1557.285	-50.839
1700	973.819	1799.440	1148.413	1106.746	448.673	1626.623	-49.979
1800	983.544	1855.384	1186.147	1204.625	451.084	1695.886	-49.212
1900	992.062	1908.794	1222.787	1303.415	453.485	1764.960	-48.521
2000	999.558	1959.875	1258.373	1403.003	455.822	1833.936	-47.897
2100	1006.180	2008.807	1292.951	1503.297	458.016	1902.784	-47.328
2200	1012.056	2055.753	1326.564	1604.215	460.065	1971.534	-46.809
2300	1017.288	2100.858	1359.255	1705.687	461.966	2040.193	-46.333
2400	1021.964	2144.254	1391.065	1807.654	463.645	2108.724	-45.894
2500	1026.158	2186.059	1422.034	1910.064	465.114	2177.306	-45.491
2600	1029.933	2226.381	1452.200	2012.871	466.338	2245.714	-45.116
2700	1033.339	2265.316	1481.598	2116.038	467.321	2314.154	-44.769
2800	1036.424	2302.953	1510.264	2219.529	468.035	2382.584	-44.447
2900	1039.225	2339.372	1538.229	2323.313	468.452	2450.939	-44.145
3000	1041.774	2374.647	1565.525	2427.365	468.616	2519.312	-43.864
3100	1044.102	2408.845	1592.180	2531.661	468.447	2587.605	-43.600
3200	1046.231	2442.028	1618.222	2636.179	467.990	2655.984	-43.354
3300	1048.185	2474.252	1643.676	2740.901	467.224	2724.423	-43.123
3400	1049.980	2505.571	1668.568	2845.811	466.121	2792.800	-42.905
3500	1051.634	2536.031	1692.919	2950.892	464.687	2861.195	-42.700
3600	1053.160	2565.678	1716.753	3056.133	462.944	2929.727	-42.508
3700	1054.572	2594.553	1740.088	3161.521	460.859	2998.329	-42.328
3800	1055.880	2622.695	1762.946	3267.044	458.407	3066.930	-42.157
3900	1057.095	2650.138	1785.344	3372.694	455.628	3135.546	-41.995
4000	1058.224	2676.915	1807.300	3478.460	452.507	3204.382	-41.844
4100	1059.275	2703.059	1828.830	3584.336	449.007	3273.223	-41.701
4200	1060.256	2728.597	1849.951	3690.313	445.156	3342.145	-41.565
4300	1061.172	2753.556	1870.676	3796.385	440.940	3411.071	-41.435
4400	1062.029	2777.961	1891.019	3902.545	436.368	3480.194	-41.314
4500	1062.832	2801.837	1910.995	4008.789	431.456	3549.481	-41.200
4600	1063.585	2825.206	1930.616	4115.110	426.149	3618.891	-41.093
4700	1064.293	2848.087	1949.895	4221.504	420.463	3688.303	-40.990
4800	1064.958	2870.501	1968.841	4327.967	414.446	3757.948	-40.894
4900	1065.585	2892.466	1987.467	4434.495	408.021	3827.584	-40.802
5000	1066.175	2914.000	2005.783	4541.083	401.286	3897.546	-40.717

3.332. Benzo[*p*]naphtho[1,8,7-*ghi*]chrysene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 385-14-8
Point Group: C₂

Length: 12.92 Å
Width: 11.43 Å
Breadth: 4.809 Å
L/B Ratio: 1.130

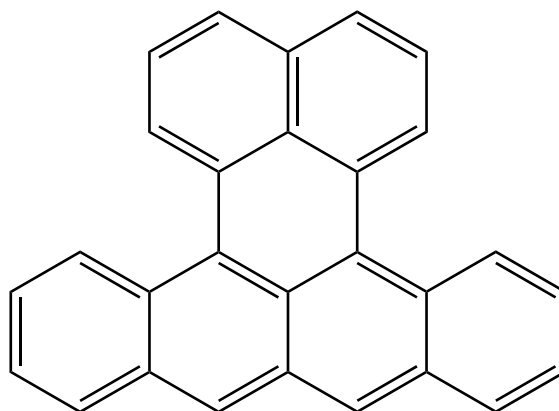
Cartesian coordinates:

C	-3.3942	2.7884	-0.0872	C	0.3464	-0.6940	-0.0325	H	-2.2643	4.5119	-0.7048
C	-1.0166	2.7700	-0.4911	C	1.6099	1.4092	0.0837	H	-5.4896	1.2455	0.5783
C	-2.2320	3.4470	-0.4506	C	2.8151	0.7235	-0.1561	H	-5.4890	-1.2438	0.5866
C	-3.3576	1.4088	0.1439	C	4.0286	1.4377	-0.2422	H	-4.3424	-3.3321	0.0064
C	-4.5693	0.6762	0.4056	C	4.0743	2.7866	0.0261	H	-2.2643	-4.5160	-0.6821
C	-4.5690	-0.6751	0.4097	C	2.9051	3.4444	0.4282	H	-0.1237	-3.3346	-0.7846
C	-3.3572	-1.4088	0.1517	C	1.7055	2.7675	0.4578	H	4.9468	0.8890	-0.5016
C	-3.3936	-2.7898	-0.0715	C	2.8154	-0.7215	-0.1596	H	5.0170	3.3383	-0.0436
C	-2.2321	-3.4495	-0.4348	C	1.6111	-1.4084	0.0828	H	2.9487	4.4995	0.7179
C	-1.0173	-2.7719	-0.4826	C	1.7094	-2.7673	0.4538	H	0.8062	3.3062	0.7859
C	-2.1291	0.7157	0.0631	C	2.9088	-3.4445	0.4137	H	0.8125	-3.3071	0.7863
C	-2.1289	-0.7158	0.0660	C	4.0751	-2.7856	0.0054	H	2.9540	-4.5007	0.6990
C	-0.9174	-1.4187	-0.1472	C	4.0282	-1.4352	-0.2558	H	5.0171	-3.3371	-0.0746
C	-0.9175	1.4180	-0.1507	H	-4.3433	3.3310	-0.0158	H	4.9453	-0.8854	-0.5166
C	0.3460	0.6935	-0.0334	H	-0.1220	3.3313	-0.7930				

Table 3.332: Table of thermodynamic data as a function of temperature for Benzo[*p*]naphtho[1,8,7-*ghi*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.434	506.587	506.587	∞
100	111.244	343.607	790.532	-44.692	533.387	582.273	-304.142
200	223.641	453.418	594.461	-28.208	519.191	636.826	-166.318
250	288.476	510.236	571.904	-15.417	512.526	667.005	-139.360
298.15	351.761	566.469	566.469	0.000	506.587	697.311	-122.164
300	354.165	568.652	566.475	0.653	506.368	698.493	-121.616
350	417.439	628.046	571.021	19.958	500.894	730.959	-109.087
400	476.188	687.680	581.878	42.321	496.144	764.149	-99.786
450	529.442	746.897	596.930	67.485	492.036	797.901	-92.616
500	577.053	805.192	614.851	95.171	488.482	832.102	-86.927
600	656.867	917.746	656.037	157.026	482.721	901.397	-78.472
700	719.932	1023.925	701.087	225.986	478.534	971.535	-72.495
800	770.464	1123.477	747.732	300.596	475.731	1042.159	-68.045
900	811.611	1216.680	794.716	379.767	474.131	1113.055	-64.599
1000	845.583	1304.005	841.325	462.679	473.567	1184.086	-61.849
1100	873.939	1385.967	887.151	548.697	473.840	1255.141	-59.600
1200	897.818	1463.063	931.964	637.318	474.810	1326.120	-57.723
1300	918.073	1535.748	975.640	728.140	476.291	1397.009	-56.131
1400	935.364	1604.434	1018.124	820.834	478.154	1467.772	-54.762
1500	950.211	1669.486	1059.399	915.132	480.315	1538.393	-53.571
1600	963.029	1731.231	1099.475	1010.809	482.644	1608.854	-52.523
1700	974.150	1789.955	1138.378	1107.681	485.068	1679.142	-51.593
1800	983.847	1845.917	1176.144	1205.592	487.511	1749.352	-50.764
1900	992.342	1899.343	1212.812	1304.410	489.942	1819.373	-50.017
2000	999.815	1950.438	1248.425	1404.026	492.305	1889.293	-49.342
2100	1006.419	1999.382	1283.028	1504.344	494.524	1959.084	-48.729
2200	1012.276	2046.339	1316.664	1605.285	496.596	2028.776	-48.168
2300	1017.493	2091.453	1349.376	1706.778	498.517	2098.376	-47.655
2400	1022.155	2134.858	1381.206	1808.765	500.216	2167.847	-47.181
2500	1026.336	2176.671	1412.193	1911.193	501.704	2237.368	-46.746
2600	1030.099	2216.999	1442.376	2014.018	502.945	2306.714	-46.342
2700	1033.495	2255.940	1471.791	2117.201	503.944	2376.092	-45.967
2800	1036.570	2293.582	1500.473	2220.707	504.674	2445.460	-45.620
2900	1039.362	2330.006	1528.453	2324.505	505.105	2514.752	-45.295
3000	1041.904	2365.286	1555.762	2428.571	505.282	2584.061	-44.992
3100	1044.223	2399.488	1582.430	2532.879	505.126	2653.290	-44.707
3200	1046.346	2432.675	1608.484	2637.409	504.680	2722.604	-44.441
3300	1048.293	2464.903	1633.950	2742.142	503.925	2791.978	-44.192
3400	1050.083	2496.224	1658.853	2847.062	502.833	2861.290	-43.957
3500	1051.731	2526.688	1683.215	2952.154	501.409	2930.620	-43.736
3600	1053.253	2556.337	1707.059	3057.404	499.675	3000.086	-43.529
3700	1054.660	2585.215	1730.404	3162.801	497.600	3069.622	-43.334
3800	1055.964	2613.358	1753.271	3268.333	495.156	3139.156	-43.150
3900	1057.174	2640.803	1775.678	3373.990	492.386	3208.707	-42.975
4000	1058.300	2667.583	1797.642	3479.765	489.272	3278.475	-42.812
4100	1059.348	2693.728	1819.180	3585.648	485.779	3348.250	-42.656
4200	1060.325	2719.268	1840.308	3691.632	481.935	3418.105	-42.509
4300	1061.238	2744.229	1861.040	3797.711	477.726	3487.964	-42.369
4400	1062.093	2768.636	1881.391	3903.878	473.161	3558.019	-42.238
4500	1062.893	2792.513	1901.374	4010.127	468.255	3628.239	-42.115
4600	1063.644	2815.883	1921.001	4116.455	462.954	3698.581	-41.998
4700	1064.349	2838.765	1940.286	4222.854	457.274	3768.925	-41.886
4800	1065.012	2861.181	1959.238	4329.323	451.262	3839.503	-41.781
4900	1065.636	2883.147	1977.870	4435.856	444.843	3910.070	-41.681
5000	1066.225	2904.682	1996.192	4542.449	438.112	3980.965	-41.588

3.333. Dibenzo[*a,f*]perylene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 191-29-7
Point Group: C₂

Length: 13.79 Å
Width: 11.76 Å
Breadth: 5.175 Å
L/B Ratio: 1.173

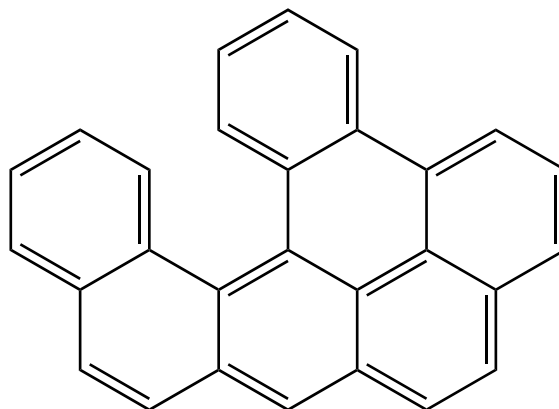
Cartesian coordinates:

C	2.4026	-3.5571	0.1936	C	0.0004	2.1166	0.4873	H	1.2012	-5.3349	0.0822
C	2.4074	-2.1498	0.1958	C	2.4001	2.2085	0.2368	H	-3.3788	-1.6494	0.3284
C	1.2224	-4.2393	0.0962	C	2.4109	0.8285	-0.1404	H	-3.3559	-4.0909	0.2839
C	-0.0010	-3.5220	0.0504	C	3.6303	0.3418	-0.7279	H	-1.2043	-5.3340	0.0856
C	-2.4084	-2.1482	0.2006	C	4.7510	1.1046	-0.8006	H	-1.2041	3.8683	0.9239
C	-2.4044	-3.5555	0.1993	C	4.7624	2.4340	-0.2835	H	1.2053	3.8673	0.9259
C	-1.2249	-4.2385	0.0992	C	3.6197	2.9714	0.2091	H	3.6407	-0.6710	-1.1535
C	-0.0006	-2.1083	0.0180	C	-2.4105	0.8294	-0.1405	H	5.6624	0.7162	-1.2672
C	1.2481	-1.4108	0.0452	C	-2.3991	2.2098	0.2352	H	5.6950	3.0064	-0.3113
C	-1.2488	-1.4101	0.0471	C	-3.6180	2.9735	0.2057	H	3.5930	4.0011	0.5839
C	-1.2490	0.0527	0.0328	C	-4.7609	2.4361	-0.2866	H	-3.5909	4.0038	0.5787
C	-1.2138	2.8193	0.6024	C	-4.7503	1.1058	-0.8013	H	-5.6928	3.0094	-0.3159
C	0.0002	0.7200	0.2077	C	-3.6301	0.3424	-0.7272	H	-5.6618	0.7169	-1.2674
C	1.2491	0.0522	0.0322	H	3.3540	-4.0931	0.2757	H	-3.6408	-0.6713	-1.1509
C	1.2152	2.8186	0.6036	H	3.3788	-1.6523	0.3218				

Table 3.333: Table of thermodynamic data as a function of temperature for Dibenzo[*a,f*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-51.684	566.070	566.070	∞
100	111.705	343.072	792.728	-44.966	592.597	641.537	-335.098
200	225.091	453.537	595.446	-28.382	578.501	696.112	-181.802
250	290.270	510.717	572.752	-15.509	571.918	726.276	-151.744
298.15	353.746	567.285	567.285	0.000	566.070	756.551	-132.542
300	356.155	569.480	567.292	0.657	565.855	757.731	-131.930
350	419.483	629.187	571.862	20.064	560.482	790.148	-117.921
400	478.191	689.092	582.774	42.527	555.834	823.274	-107.506
450	531.350	748.540	597.896	67.790	551.824	856.949	-99.470
500	578.841	807.030	615.895	95.568	548.362	891.063	-93.087
600	658.407	919.888	657.240	157.589	542.768	960.159	-83.588
700	721.254	1026.287	702.441	226.692	538.723	1030.070	-76.863
800	771.607	1126.003	749.222	301.425	536.043	1100.450	-71.851
900	812.609	1219.332	796.329	380.703	534.550	1171.087	-67.967
1000	846.462	1306.756	843.047	463.709	534.080	1241.847	-64.866
1100	874.720	1388.798	888.971	549.810	534.436	1312.623	-62.330
1200	898.515	1465.957	933.870	638.505	535.479	1383.316	-60.213
1300	918.699	1538.696	977.625	729.392	537.027	1453.912	-58.418
1400	935.928	1607.426	1020.178	822.146	538.948	1524.378	-56.874
1500	950.722	1672.515	1061.517	916.497	541.163	1594.699	-55.531
1600	963.493	1734.291	1101.652	1012.223	543.542	1664.855	-54.351
1700	974.574	1793.043	1140.608	1109.139	546.010	1734.836	-53.304
1800	984.235	1849.027	1178.422	1207.091	548.493	1804.736	-52.371
1900	992.697	1902.474	1215.134	1305.946	550.961	1874.444	-51.531
2000	1000.143	1953.586	1250.788	1405.596	553.359	1944.051	-50.772
2100	1006.721	2002.546	1285.428	1505.946	555.609	2013.526	-50.083
2200	1012.556	2049.516	1319.099	1606.916	557.710	2082.901	-49.453
2300	1017.752	2094.642	1351.844	1708.436	559.658	2152.182	-48.877
2400	1022.396	2138.057	1383.704	1810.448	561.382	2221.334	-48.345
2500	1026.561	2179.880	1414.720	1912.899	562.894	2290.535	-47.857
2600	1030.309	2220.216	1444.929	2015.746	564.156	2359.560	-47.403
2700	1033.691	2259.165	1474.369	2118.949	565.175	2428.615	-46.983
2800	1036.754	2296.814	1503.074	2222.474	565.924	2497.660	-46.593
2900	1039.535	2333.244	1531.075	2326.290	566.373	2566.629	-46.229
3000	1042.066	2368.530	1558.406	2430.372	566.567	2635.614	-45.889
3100	1044.377	2402.737	1585.093	2534.696	566.426	2704.518	-45.570
3200	1046.491	2435.929	1611.166	2639.241	565.995	2773.507	-45.272
3300	1048.430	2468.161	1636.649	2743.988	565.255	2842.555	-44.993
3400	1050.212	2499.486	1661.568	2848.922	564.176	2911.541	-44.729
3500	1051.854	2529.954	1685.946	2954.026	562.765	2980.545	-44.481
3600	1053.369	2559.607	1709.804	3059.288	561.043	3049.684	-44.249
3700	1054.771	2588.487	1733.164	3164.696	558.979	3118.893	-44.030
3800	1056.069	2616.634	1756.044	3270.239	556.545	3188.100	-43.823
3900	1057.274	2644.081	1778.464	3375.907	553.785	3257.323	-43.626
4000	1058.395	2670.863	1800.441	3481.691	550.681	3326.764	-43.442
4100	1059.439	2697.011	1821.991	3587.583	547.198	3396.210	-43.267
4200	1060.412	2722.553	1843.130	3693.576	543.363	3465.737	-43.102
4300	1061.322	2747.515	1863.873	3799.664	539.162	3535.267	-42.944
4400	1062.172	2771.925	1884.234	3905.839	534.605	3604.993	-42.796
4500	1062.969	2795.804	1904.227	4012.096	529.707	3674.884	-42.656
4600	1063.717	2819.175	1923.864	4118.431	524.413	3744.897	-42.524
4700	1064.419	2842.059	1943.157	4224.838	518.741	3814.912	-42.397
4800	1065.079	2864.476	1962.119	4331.313	512.736	3885.160	-42.278
4900	1065.701	2886.443	1980.759	4437.853	506.323	3955.398	-42.164
5000	1066.287	2907.979	1999.089	4544.452	499.599	4025.963	-42.058

3.334. Tribenzo[*c,g,mno*]chrysene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 108650-10-8
Point Group: C₁

Length: 14.17 Å
Width: 11.60 Å
Breadth: 6.227 Å
L/B Ratio: 1.222

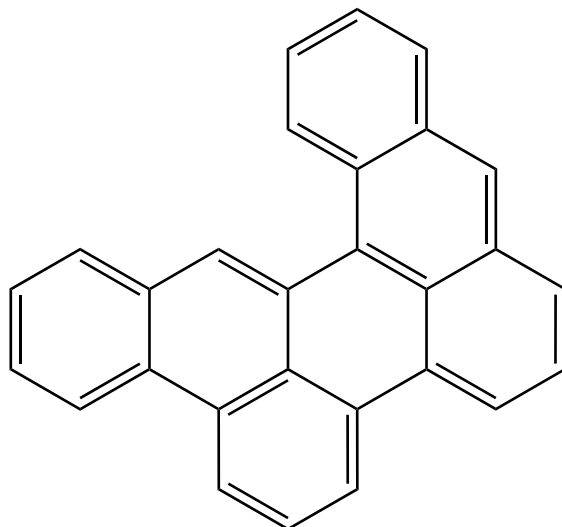
Cartesian coordinates:

C	0.7928	2.0838	1.0466	C	0.2449	-2.9402	0.5168	H	1.7456	1.6320	1.3525
C	2.5232	1.0729	-1.0468	C	-2.4085	-0.4003	-0.1197	H	3.6712	2.5793	-2.0574
C	2.5339	-0.1106	-0.2768	C	-3.5243	-1.2397	-0.3256	H	4.7997	-2.4772	0.7837
C	1.3094	-0.7668	0.1521	C	-3.3729	-2.6657	-0.1777	H	2.7004	-3.7808	1.0809
C	0.0313	-0.1504	0.2206	C	-2.1710	-3.2066	0.1157	H	0.3321	-4.0126	0.7304
C	-0.1901	1.2747	0.4455	C	-2.5673	0.9997	-0.1992	H	-2.0524	-4.2892	0.2395
C	3.7754	-0.7291	-0.0331	C	-3.8088	1.5309	-0.5511	H	-4.2612	-3.2946	-0.3076
C	4.9720	-0.0973	-0.4296	C	-4.8936	0.6945	-0.7943	H	-5.6234	-1.3349	-0.8388
C	4.9341	1.0902	-1.1254	C	-4.7614	-0.6800	-0.6681	H	-5.8593	1.1276	-1.0754
C	3.6980	1.6615	-1.4608	C	-1.4468	1.8468	0.1735	H	-3.9196	2.6241	-0.6157
C	1.3974	-2.1456	0.4584	C	0.5762	3.4315	1.2601	H	-2.6155	3.6606	0.0903
C	2.6800	-2.7462	0.7192	C	-0.6356	4.0164	0.8821	H	-0.7927	5.0906	1.0226
C	3.8216	-2.0456	0.5431	C	-1.6391	3.2274	0.3572	H	1.3551	4.0442	1.7258
C	-1.1112	-0.9709	0.1329	H	5.8618	1.5814	-1.4359	H	1.5610	1.5220	-1.3257
C	-0.9976	-2.3795	0.2535	H	5.9309	-0.5725	-0.1929				

Table 3.334: Table of thermodynamic data as a function of temperature for Tribenzo[*c,g,mno*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.564	487.195	487.195	∞
100	111.434	350.233	798.049	-44.782	513.905	562.129	-293.620
200	224.109	460.204	601.568	-28.273	499.734	616.011	-160.882
250	289.154	517.150	578.959	-15.452	493.098	645.849	-134.940
298.15	352.526	573.512	573.512	0.000	487.195	675.819	-118.398
300	354.931	575.700	573.518	0.654	486.977	676.987	-117.872
350	418.197	635.212	578.074	19.998	481.541	709.098	-105.825
400	476.887	694.944	588.951	42.397	476.828	741.927	-96.884
450	530.064	754.239	604.029	67.595	472.753	775.314	-89.994
500	577.599	812.596	621.977	95.309	469.228	809.146	-84.529
600	657.294	925.238	663.217	157.213	463.515	877.696	-76.409
700	720.287	1031.476	708.316	226.212	459.367	947.082	-70.671
800	770.779	1131.073	755.004	300.855	456.597	1016.949	-66.399
900	811.902	1224.311	802.026	380.056	455.027	1087.083	-63.091
1000	845.858	1311.666	848.670	462.997	454.492	1157.349	-60.452
1100	874.202	1393.654	894.526	549.041	454.792	1227.636	-58.294
1200	898.068	1470.772	939.365	637.688	455.787	1297.846	-56.493
1300	918.311	1543.477	983.066	728.535	457.293	1367.963	-54.964
1400	935.590	1612.180	1025.572	821.252	459.179	1437.952	-53.650
1500	950.424	1677.248	1066.867	915.571	461.362	1507.798	-52.505
1600	963.230	1739.005	1106.962	1011.269	463.712	1577.482	-51.498
1700	974.339	1797.742	1145.883	1108.161	466.155	1646.992	-50.605
1800	984.025	1853.714	1183.664	1206.090	468.616	1716.423	-49.808
1900	992.509	1907.150	1220.347	1304.926	471.064	1785.663	-49.090
2000	999.972	1958.253	1255.974	1404.558	473.444	1854.803	-48.441
2100	1006.566	2007.204	1290.590	1504.891	475.678	1923.812	-47.851
2200	1012.415	2054.167	1324.238	1605.846	477.764	1992.721	-47.312
2300	1017.623	2099.288	1356.961	1707.353	479.699	2061.538	-46.818
2400	1022.277	2142.698	1388.801	1809.352	481.411	2130.225	-46.362
2500	1026.451	2184.515	1419.799	1911.792	482.911	2198.962	-45.944
2600	1030.207	2224.848	1449.991	2014.628	484.163	2267.523	-45.554
2700	1033.597	2263.793	1479.415	2117.821	485.172	2336.116	-45.194
2800	1036.667	2301.439	1508.104	2221.337	485.912	2404.699	-44.859
2900	1039.453	2337.866	1536.092	2325.145	486.352	2473.205	-44.546
3000	1041.990	2373.149	1563.409	2429.219	486.538	2541.727	-44.254
3100	1044.305	2407.354	1590.084	2533.536	486.391	2610.170	-43.980
3200	1046.424	2440.543	1616.145	2638.074	485.953	2678.698	-43.724
3300	1048.367	2472.774	1641.617	2742.815	485.206	2747.284	-43.485
3400	1050.153	2504.097	1666.526	2847.742	484.121	2815.809	-43.259
3500	1051.798	2534.563	1690.894	2952.841	482.703	2884.352	-43.046
3600	1053.316	2564.214	1714.743	3058.098	480.976	2953.030	-42.846
3700	1054.721	2593.094	1738.093	3163.500	478.907	3021.778	-42.659
3800	1056.022	2621.239	1760.965	3269.038	476.469	3090.525	-42.481
3900	1057.230	2648.685	1783.377	3374.702	473.704	3159.287	-42.313
4000	1058.352	2675.466	1805.346	3480.481	470.596	3228.267	-42.156
4100	1059.398	2701.613	1826.888	3586.369	467.108	3297.254	-42.007
4200	1060.373	2727.153	1848.020	3692.359	463.269	3366.320	-41.865
4300	1061.285	2752.115	1868.757	3798.442	459.065	3435.390	-41.731
4400	1062.137	2776.524	1889.111	3904.614	454.504	3504.657	-41.605
4500	1062.936	2800.402	1909.098	4010.868	449.602	3574.088	-41.486
4600	1063.685	2823.772	1928.729	4117.199	444.306	3643.641	-41.374
4700	1064.388	2846.656	1948.017	4223.603	438.630	3713.196	-41.267
4800	1065.050	2869.072	1966.973	4330.075	432.622	3782.985	-41.166
4900	1065.673	2891.039	1985.608	4436.612	426.206	3852.763	-41.070
5000	1066.260	2912.574	2003.932	4543.209	419.479	3922.868	-40.981

3.335. Dibenzo[*a,n*]perylene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 191-81-1
Point Group: C₁

Length: 13.95 Å
Width: 11.51 Å
Breadth: 5.224 Å
L/B Ratio: 1.211

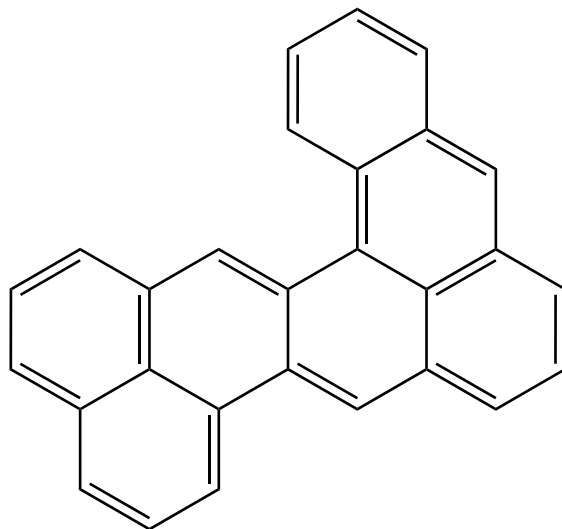
Cartesian coordinates:

C	1.3082	-2.7079	-0.6069	C	-3.2320	-0.1929	-0.0007	H	-5.1633	0.6975	-0.3988
C	1.8574	-1.4572	-0.1708	C	-2.5465	-1.3577	0.3796	H	-2.7378	-3.4292	0.9996
C	3.2675	-1.4138	0.0283	C	-1.1153	-1.3649	0.4125	H	-0.6273	-2.3134	0.6816
C	4.0472	-2.6112	-0.0925	C	-4.6400	-0.2209	-0.0918	H	1.2207	4.3436	0.1317
C	3.4693	-3.7828	-0.4662	C	-5.3364	-1.3702	0.2041	H	3.6563	4.3619	0.6240
C	2.0771	-3.8208	-0.7528	C	-4.6504	-2.5293	0.6046	H	4.9269	2.2213	0.7205
C	3.9036	-0.2094	0.3269	C	-3.2771	-2.5263	0.6910	H	-4.2232	2.2115	-0.6658
C	3.1769	0.9811	0.3399	C	3.8467	2.2305	0.5356	H	-2.9243	4.3281	-0.9325
C	1.7690	0.9508	0.1488	C	3.1535	3.4001	0.4803	H	-0.4611	4.3303	-0.5407
C	1.0913	-0.2812	0.0169	C	1.7602	3.3879	0.2207	H	4.9838	-0.1928	0.5191
C	1.0769	2.2081	0.0638	C	-1.0287	3.3884	-0.4922	H	5.1223	-2.5540	0.1138
C	-0.3564	2.2072	-0.2110	C	-2.4131	3.3910	-0.6894	H	4.0589	-4.6998	-0.5641
C	-1.0691	0.9860	-0.1417	C	-3.1282	2.2221	-0.5523	H	1.6358	-4.7610	-1.0999
C	-0.3753	-0.2629	0.0876	H	-5.2171	-3.4346	0.8453	H	0.2364	-2.7604	-0.8436
C	-2.4731	1.0113	-0.2490	H	-6.4287	-1.3873	0.1320				

Table 3.335: Table of thermodynamic data as a function of temperature for Dibenzo[*a,n*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-51.882	499.882	499.882	∞
100	112.925	353.150	803.182	-45.003	526.371	574.303	-299.979
200	225.201	464.089	605.875	-28.357	512.337	627.838	-163.971
250	289.996	521.251	583.206	-15.489	505.750	657.475	-137.369
298.15	353.212	577.746	577.746	0.000	499.882	687.244	-120.400
300	355.613	579.938	577.753	0.656	499.666	688.405	-119.859
350	418.775	639.547	582.316	20.031	494.261	720.301	-107.497
400	477.392	699.351	593.209	42.457	489.575	752.911	-98.318
450	530.514	758.703	608.307	67.678	485.524	786.076	-91.243
500	578.003	817.104	626.276	95.414	482.020	819.684	-85.630
600	657.621	929.813	667.557	157.354	476.344	887.780	-77.287
700	720.549	1036.097	712.693	226.382	472.225	956.705	-71.389
800	770.985	1135.725	759.414	301.049	469.479	1026.109	-66.997
900	812.064	1228.985	806.464	380.269	467.927	1095.777	-63.596
1000	845.984	1316.355	853.132	463.223	467.406	1165.575	-60.882
1100	874.300	1398.354	899.009	549.279	467.717	1235.392	-58.663
1200	898.144	1475.479	943.867	637.935	468.721	1305.132	-56.810
1300	918.370	1548.189	987.583	728.788	470.234	1374.777	-55.238
1400	935.635	1616.896	1030.103	821.510	472.124	1444.295	-53.886
1500	950.460	1681.967	1071.411	915.833	474.312	1513.670	-52.710
1600	963.257	1743.726	1111.517	1011.535	476.665	1582.882	-51.675
1700	974.361	1802.464	1150.448	1108.428	479.111	1651.920	-50.756
1800	984.042	1858.438	1188.238	1206.359	481.574	1720.878	-49.938
1900	992.521	1911.874	1224.929	1305.197	484.023	1789.646	-49.200
2000	999.982	1962.978	1260.563	1404.830	486.404	1858.313	-48.533
2100	1006.573	2011.930	1295.185	1505.164	488.638	1926.850	-47.927
2200	1012.420	2058.893	1328.839	1606.119	490.726	1995.286	-47.373
2300	1017.627	2104.014	1361.567	1707.627	492.661	2063.630	-46.866
2400	1022.280	2147.424	1393.413	1809.626	494.373	2131.845	-46.397
2500	1026.453	2189.241	1424.415	1912.067	495.873	2200.109	-45.968
2600	1030.208	2229.574	1454.611	2014.903	497.125	2268.198	-45.568
2700	1033.598	2268.519	1484.039	2118.096	498.135	2336.318	-45.198
2800	1036.667	2306.165	1512.732	2221.612	498.874	2404.428	-44.854
2900	1039.453	2342.592	1540.723	2325.420	499.315	2472.462	-44.533
3000	1041.989	2377.875	1568.043	2429.494	499.501	2540.512	-44.233
3100	1044.305	2412.080	1594.722	2533.811	499.353	2608.482	-43.952
3200	1046.423	2445.269	1620.785	2638.349	498.915	2676.537	-43.689
3300	1048.366	2477.499	1646.260	2743.090	498.168	2744.651	-43.443
3400	1050.152	2508.823	1671.171	2848.017	497.083	2812.703	-43.211
3500	1051.797	2539.289	1695.541	2953.115	495.665	2880.773	-42.992
3600	1053.315	2568.940	1719.392	3058.372	493.938	2948.979	-42.788
3700	1054.719	2597.819	1742.745	3163.774	491.869	3017.254	-42.595
3800	1056.020	2625.964	1765.619	3269.312	489.430	3085.528	-42.413
3900	1057.228	2653.411	1788.032	3374.975	486.666	3153.818	-42.240
4000	1058.351	2680.192	1810.003	3480.755	483.557	3222.326	-42.078
4100	1059.397	2706.338	1831.547	3586.643	480.069	3290.840	-41.925
4200	1060.372	2731.879	1852.681	3692.632	476.230	3359.434	-41.780
4300	1061.283	2756.841	1873.419	3798.715	472.025	3428.031	-41.641
4400	1062.136	2781.249	1893.775	3904.887	467.465	3496.825	-41.512
4500	1062.934	2805.127	1913.763	4011.140	462.563	3565.784	-41.390
4600	1063.683	2828.498	1933.395	4117.472	457.266	3634.864	-41.274
4700	1064.387	2851.381	1952.684	4223.876	451.590	3703.947	-41.164
4800	1065.048	2873.797	1971.641	4330.348	445.582	3773.263	-41.061
4900	1065.671	2895.764	1990.278	4436.884	439.166	3842.568	-40.961
5000	1066.258	2917.300	2008.603	4543.481	432.439	3912.201	-40.870

3.336. Benzo[de]naphtho[3,2,1-mn]naphthacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-45-2
Point Group: C₁

Length: 14.41 Å
Width: 11.69 Å
Breadth: 5.480 Å
L/B Ratio: 1.233

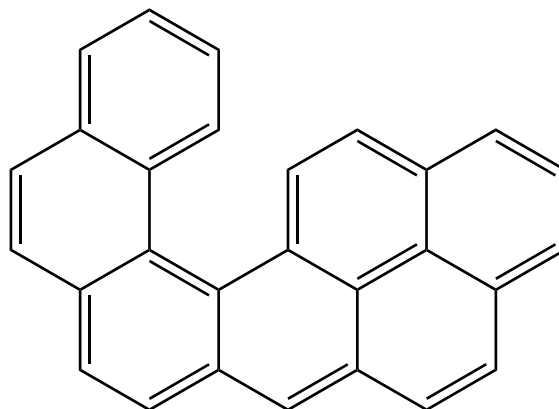
Cartesian coordinates:

C	5.0806	-1.1107	0.4997	C	-1.9496	-3.5089	-0.2608	H	2.3922	-3.1427	1.0102
C	4.3637	-2.2219	0.8568	C	-3.3506	-3.5328	-0.4706	H	2.5253	3.2264	-1.2360
C	2.9568	-2.2331	0.7548	C	-4.0654	-2.3726	-0.4742	H	5.0006	3.2041	-1.1486
C	4.4111	0.0513	0.0303	C	-2.0013	-1.0685	-0.1328	H	6.2187	1.2044	-0.3191
C	3.0415	2.3262	-0.8835	C	-3.4128	-1.1151	-0.2795	H	0.3846	2.1764	-0.7440
C	4.4492	2.3138	-0.8280	C	-4.1506	0.0684	-0.2270	H	0.6625	-3.2388	0.3167
C	5.1242	1.2094	-0.3734	C	-1.3280	0.1667	-0.0011	H	-1.4001	-4.4564	-0.2260
C	2.3186	1.2175	-0.4888	C	-2.0981	1.3368	0.1990	H	-3.8474	-4.4973	-0.6186
C	3.0034	0.0513	-0.0439	C	-3.5144	1.2781	0.0495	H	-5.1517	-2.3807	-0.6196
C	2.2740	-1.1189	0.3135	C	-4.2997	2.4694	0.1949	H	-5.2372	0.0414	-0.3768
C	0.8715	1.2290	-0.4687	C	-3.7184	3.6492	0.5356	H	-5.3820	2.4009	0.0341
C	0.1382	0.1522	-0.0897	C	-2.3152	3.7048	0.7601	H	-4.3132	4.5606	0.6525
C	0.8201	-1.1207	0.1543	C	-1.5421	2.5978	0.5947	H	-1.8684	4.6540	1.0742
C	0.1341	-2.2870	0.1451	H	6.1742	-1.1014	0.5677	H	-0.4606	2.6629	0.7792
C	-1.2889	-2.3160	-0.0971	H	4.8753	-3.1190	1.2208				

Table 3.336: Table of thermodynamic data as a function of temperature for Benzo[*de*]naphtho[3,2,1-*mn*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.910	530.849	530.849	∞
100	112.295	353.189	803.921	-45.073	557.267	605.196	-316.115
200	225.644	463.988	606.194	-28.441	543.220	658.740	-172.042
250	290.894	521.301	583.454	-15.538	536.666	688.379	-143.826
298.15	354.340	577.977	577.977	0.000	530.849	718.141	-125.813
300	356.747	580.177	577.984	0.658	530.635	719.302	-125.239
350	419.981	639.967	582.562	20.092	525.289	751.182	-112.105
400	478.578	699.932	593.487	42.578	520.663	783.767	-102.347
450	531.635	759.419	608.626	67.857	516.670	816.899	-94.821
500	579.044	817.935	626.641	95.647	513.220	850.468	-88.846
600	658.508	930.820	668.015	157.683	507.640	918.472	-79.958
700	721.315	1037.231	713.239	226.794	503.603	987.290	-73.671
800	771.661	1136.954	760.039	301.532	500.929	1056.575	-68.986
900	812.671	1230.290	807.161	380.816	499.441	1126.116	-65.357
1000	846.535	1317.721	853.893	463.829	498.977	1195.780	-62.460
1100	874.803	1399.770	899.827	549.937	499.342	1265.459	-60.090
1200	898.606	1476.937	944.737	638.641	500.394	1335.054	-58.112
1300	918.794	1549.683	988.500	729.538	501.951	1404.552	-56.434
1400	936.027	1618.420	1031.062	822.301	503.882	1473.919	-54.991
1500	950.821	1683.517	1072.409	916.662	506.107	1543.140	-53.736
1600	963.590	1745.299	1112.550	1012.398	508.495	1612.196	-52.632
1700	974.669	1804.056	1151.513	1109.324	510.973	1681.075	-51.652
1800	984.327	1860.046	1189.333	1207.285	513.465	1749.874	-50.779
1900	992.786	1913.498	1226.051	1306.149	515.942	1818.480	-49.992
2000	1000.228	1964.614	1261.710	1405.808	518.349	1886.984	-49.282
2100	1006.802	2013.578	1296.356	1506.166	520.607	1955.356	-48.636
2200	1012.633	2060.552	1330.032	1607.144	522.716	2023.627	-48.046
2300	1017.826	2105.682	1362.781	1708.671	524.672	2091.805	-47.505
2400	1022.466	2149.100	1394.646	1810.690	526.403	2159.853	-47.007
2500	1026.628	2190.925	1425.665	1913.149	527.921	2227.949	-46.549
2600	1030.372	2231.264	1455.879	2016.002	529.191	2295.869	-46.124
2700	1033.751	2270.215	1485.322	2119.211	530.216	2363.820	-45.730
2800	1036.811	2307.867	1514.030	2222.742	530.970	2431.760	-45.364
2900	1039.589	2344.299	1542.035	2326.564	531.424	2499.623	-45.022
3000	1042.118	2379.586	1569.369	2430.651	531.624	2567.502	-44.703
3100	1044.426	2413.795	1596.059	2534.980	531.489	2635.301	-44.404
3200	1046.538	2446.988	1622.135	2639.530	531.062	2703.185	-44.124
3300	1048.474	2479.222	1647.621	2744.282	530.326	2771.127	-43.862
3400	1050.255	2510.548	1672.543	2849.219	529.252	2839.006	-43.615
3500	1051.894	2541.017	1696.923	2954.328	527.845	2906.904	-43.382
3600	1053.408	2570.671	1720.784	3059.594	526.127	2974.937	-43.164
3700	1054.808	2599.553	1744.146	3165.006	524.066	3043.039	-42.959
3800	1056.105	2627.700	1767.028	3270.552	521.637	3111.139	-42.765
3900	1057.308	2655.149	1789.450	3376.223	518.880	3179.255	-42.580
4000	1058.428	2681.932	1811.429	3482.011	515.780	3247.589	-42.408
4100	1059.470	2708.080	1832.981	3587.906	512.299	3315.929	-42.245
4200	1060.442	2733.622	1854.122	3693.903	508.467	3384.349	-42.090
4300	1061.350	2758.586	1874.867	3799.993	504.269	3452.772	-41.942
4400	1062.200	2782.996	1895.229	3906.171	499.715	3521.391	-41.803
4500	1062.996	2806.875	1915.224	4012.431	494.820	3590.175	-41.673
4600	1063.742	2830.247	1934.863	4118.768	489.529	3659.081	-41.549
4700	1064.443	2853.132	1954.158	4225.178	483.859	3727.988	-41.431
4800	1065.103	2875.549	1973.121	4331.655	477.856	3797.129	-41.320
4900	1065.724	2897.517	1991.762	4438.197	471.446	3866.260	-41.214
5000	1066.309	2919.053	2010.094	4544.799	464.724	3935.717	-41.115

3.337. Benzo[*mno*]naphtho[2,1-*c*]chrysene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 137570-57-1
Point Group: C₁

Length: 14.27 Å
Width: 10.68 Å
Breadth: 6.226 Å
L/B Ratio: 1.337

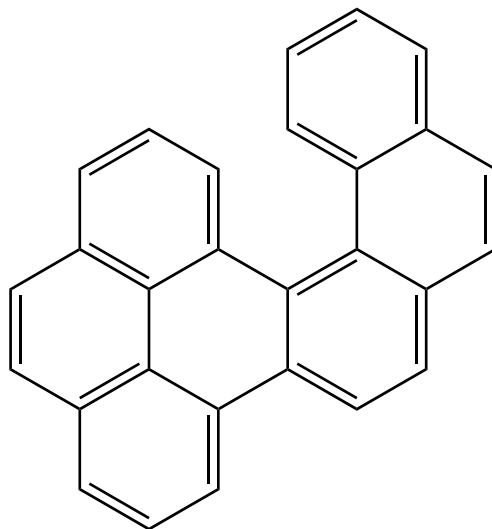
Cartesian coordinates:

C	1.8226	-1.5807	1.0359	C	-3.7369	-2.5027	-0.7998	H	-3.5765	-3.5046	-1.2134
C	-0.2762	-1.1591	-0.9006	C	-5.0028	-2.1001	-0.4116	H	-5.3656	1.6958	1.0480
C	-0.4342	0.1284	-0.2802	C	-5.2168	-0.8207	0.1031	H	-3.4741	3.2955	1.2068
C	0.6647	1.0176	-0.0681	C	-1.3258	-1.9974	-1.0858	H	-1.1329	3.8561	0.6713
C	2.0601	0.6378	-0.1126	C	2.9966	1.6192	-0.4562	H	0.8198	-1.2947	1.3795
C	2.5689	-0.6644	0.2536	C	2.6350	3.0020	-0.4350	H	-1.1876	-2.9717	-1.5683
C	0.3659	2.3841	0.1253	C	1.3855	3.3724	-0.0565	H	1.1208	4.4289	0.0658
C	-0.9465	2.7999	0.4402	C	3.8993	-1.0022	-0.0685	H	3.3990	3.7497	-0.6766
C	-1.9833	1.8905	0.4540	C	4.7609	-0.0259	-0.6597	H	5.0139	2.0389	-1.1584
C	-1.7389	0.5544	0.0220	C	4.3397	1.2581	-0.7879	H	5.7730	-0.3245	-0.9550
C	-2.8494	-0.3391	-0.1323	C	2.3426	-2.8036	1.3830	H	5.4261	-2.5435	-0.0409
C	-4.1542	0.0681	0.2409	C	3.6351	-3.1728	0.9661	H	4.0236	-4.1628	1.2255
C	-4.3518	1.4065	0.7481	C	4.4053	-2.2824	0.2606	H	1.7552	-3.4993	1.9913
C	-3.3231	2.2744	0.8380	H	-5.8487	-2.7883	-0.5123	H	0.7251	-1.4458	-1.2482
C	-2.6470	-1.6279	-0.6674	H	-6.2266	-0.5134	0.3979				

Table 3.337: Table of thermodynamic data as a function of temperature for Benzo[*mno*]naphtho[2,1-*c*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.318	484.433	484.433	∞
100	109.724	349.854	795.982	-44.613	511.312	559.574	-292.285
200	223.343	458.836	600.040	-28.241	497.004	613.555	-160.241
250	288.873	515.669	577.450	-15.445	490.344	643.464	-134.442
298.15	352.486	572.004	572.004	0.000	484.433	673.507	-117.993
300	354.898	574.192	572.011	0.654	484.215	674.678	-117.469
350	418.258	633.707	576.566	19.999	478.780	706.864	-105.492
400	476.968	693.449	587.444	42.402	474.071	739.768	-96.602
450	530.136	752.754	602.524	67.603	470.000	773.229	-89.752
500	577.656	811.117	620.475	95.321	466.478	807.136	-84.319
600	657.332	923.768	661.719	157.229	460.770	875.833	-76.247
700	720.327	1030.012	706.823	226.232	456.625	945.365	-70.543
800	770.831	1129.614	753.515	300.880	453.860	1015.379	-66.296
900	811.971	1222.860	800.541	380.087	452.296	1085.658	-63.009
1000	845.941	1310.223	847.188	463.035	451.768	1156.069	-60.386
1100	874.295	1392.219	893.048	549.089	452.078	1226.500	-58.240
1200	898.168	1469.346	937.891	637.745	453.082	1296.853	-56.449
1300	918.415	1542.059	981.596	728.602	454.599	1367.112	-54.930
1400	935.694	1610.770	1024.106	821.330	456.495	1437.243	-53.623
1500	950.528	1675.845	1065.405	915.659	458.688	1507.229	-52.485
1600	963.331	1737.609	1105.504	1011.368	461.049	1577.054	-51.484
1700	974.437	1796.351	1144.429	1108.269	463.502	1646.703	-50.596
1800	984.119	1852.329	1182.214	1206.208	465.973	1716.272	-49.804
1900	992.599	1905.770	1218.900	1305.053	468.430	1785.651	-49.090
2000	1000.058	1956.877	1254.530	1404.693	470.818	1854.928	-48.445
2100	1006.648	2005.833	1289.149	1505.035	473.060	1924.075	-47.858
2200	1012.492	2052.800	1322.801	1605.998	475.155	1993.121	-47.322
2300	1017.696	2097.924	1355.527	1707.513	477.098	2062.074	-46.830
2400	1022.347	2141.337	1387.370	1809.519	478.816	2130.898	-46.377
2500	1026.518	2183.157	1418.371	1911.966	480.323	2199.771	-45.961
2600	1030.270	2223.492	1448.566	2014.809	481.582	2268.468	-45.573
2700	1033.657	2262.439	1477.992	2118.008	482.597	2337.196	-45.215
2800	1036.723	2300.087	1506.684	2221.529	483.342	2405.914	-44.882
2900	1039.507	2336.517	1534.674	2325.343	483.788	2474.555	-44.571
3000	1042.041	2371.801	1561.994	2429.423	483.979	2543.212	-44.280
3100	1044.354	2406.008	1588.671	2533.744	483.837	2611.790	-44.007
3200	1046.470	2439.198	1614.734	2638.287	483.404	2680.452	-43.753
3300	1048.411	2471.430	1640.208	2743.032	482.661	2749.173	-43.515
3400	1050.195	2502.755	1665.119	2847.964	481.581	2817.832	-43.290
3500	1051.838	2533.222	1689.489	2953.066	480.167	2886.509	-43.078
3600	1053.355	2562.875	1713.339	3058.327	478.444	2955.321	-42.880
3700	1054.757	2591.755	1736.692	3163.734	476.379	3024.203	-42.693
3800	1056.057	2619.901	1759.565	3269.275	473.944	3093.084	-42.517
3900	1057.263	2647.348	1781.978	3374.942	471.183	3161.979	-42.349
4000	1058.384	2674.130	1803.949	3480.725	468.078	3231.094	-42.193
4100	1059.429	2700.277	1825.493	3586.616	464.593	3300.213	-42.044
4200	1060.403	2725.819	1846.626	3692.608	460.757	3369.414	-41.904
4300	1061.313	2750.781	1867.364	3798.695	456.555	3438.617	-41.770
4400	1062.164	2775.190	1887.720	3904.869	451.998	3508.017	-41.645
4500	1062.961	2799.069	1907.708	4011.126	447.098	3577.581	-41.527
4600	1063.709	2822.440	1927.340	4117.459	441.804	3647.268	-41.415
4700	1064.412	2845.324	1946.629	4223.866	436.131	3716.956	-41.308
4800	1065.073	2867.741	1965.586	4330.340	430.125	3786.878	-41.209
4900	1065.695	2889.708	1984.223	4436.879	423.712	3856.789	-41.113
5000	1066.281	2911.244	2002.548	4543.478	416.987	3927.027	-41.025

3.338. Benzo[*c*]naphtho[8,1,2-*ghi*]chrysene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 137570-60-6
Point Group: C₁

Length: 13.95 Å
Width: 10.32 Å
Breadth: 6.464 Å
L/B Ratio: 1.352

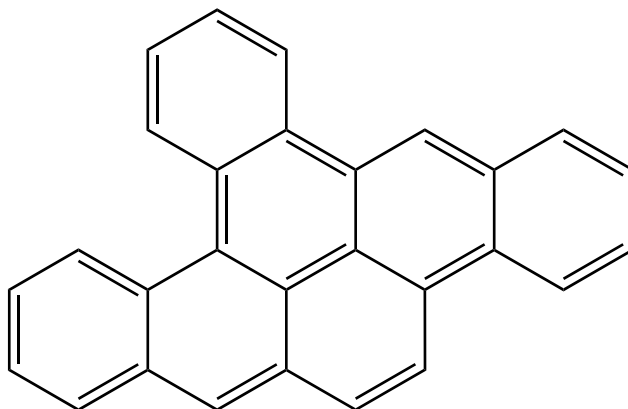
Cartesian coordinates:

C	-2.2922	1.3070	1.0444	C	2.8902	-2.5400	0.4274	H	-0.3708	3.8348	-1.7404
C	-0.3660	1.7891	-1.0658	C	4.2333	-2.3236	0.7280	H	4.1062	3.4328	-0.1517
C	0.3526	0.7469	-0.4782	C	4.7579	-1.0419	0.7258	H	5.5240	1.5371	0.6020
C	-0.2382	-0.5636	-0.2225	C	0.6238	-1.6623	-0.1194	H	5.8161	-0.8763	0.9572
C	-1.6498	-0.8025	-0.1548	C	-2.1154	-2.0937	-0.4614	H	4.8773	-3.1773	0.9640
C	-2.6369	0.1673	0.2812	C	-1.2107	-3.1799	-0.5292	H	2.4832	-3.5626	0.4156
C	1.7334	0.9450	-0.2319	C	0.1162	-2.9756	-0.2680	H	0.8189	-3.8206	-0.2053
C	2.3118	2.2203	-0.4054	C	-4.0039	-0.0856	0.0535	H	-1.5916	-4.1838	-0.7484
C	1.5373	3.2668	-0.9244	C	-4.4177	-1.3381	-0.5100	H	-3.8197	-3.3183	-1.0473
C	0.2215	3.0340	-1.2850	C	-3.5116	-2.3263	-0.6975	H	-5.4801	-1.4891	-0.7318
C	2.5720	-0.1606	0.1322	C	-3.2532	2.1979	1.4632	H	-6.0308	0.6652	0.2276
C	3.9380	0.0515	0.4130	C	-4.6044	1.9896	1.1405	H	-5.3553	2.7214	1.4552
C	4.4709	1.3867	0.3384	C	-4.9759	0.8577	0.4545	H	-2.9694	3.0744	2.0550
C	3.6974	2.4193	-0.0678	H	1.9844	4.2576	-1.0624	H	-1.4130	1.6320	-1.3569
C	2.0432	-1.4703	0.1395	H	-1.2409	1.4715	1.3143				

Table 3.338: Table of thermodynamic data as a function of temperature for Benzo[*c*]naphtho[8,1,2-*ghi*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.557	484.111	484.111	∞
100	111.115	351.694	799.185	-44.749	510.854	558.932	-291.950
200	223.951	461.444	602.799	-28.271	496.652	612.682	-160.013
250	289.150	518.373	580.190	-15.454	490.013	642.458	-134.231
298.15	352.610	574.742	574.742	0.000	484.111	672.369	-117.794
300	355.018	576.930	574.748	0.655	483.894	673.535	-117.270
350	418.328	636.460	579.305	20.004	478.463	705.584	-105.300
400	477.038	696.210	590.185	42.410	473.757	738.350	-96.417
450	530.222	755.524	605.268	67.615	469.691	771.673	-89.572
500	577.755	813.897	623.221	95.338	466.173	805.441	-84.142
600	657.435	926.567	664.473	157.256	460.475	873.859	-76.075
700	720.409	1032.825	709.585	226.269	456.340	943.111	-70.374
800	770.880	1132.437	756.284	300.922	453.582	1012.842	-66.130
900	811.986	1225.686	803.316	380.133	452.021	1082.839	-62.845
1000	845.927	1313.050	849.968	463.082	451.493	1152.967	-60.224
1100	874.259	1395.043	895.832	549.132	451.800	1223.116	-58.080
1200	898.115	1472.166	940.679	637.784	452.800	1293.187	-56.290
1300	918.350	1544.874	984.386	728.635	454.310	1363.164	-54.771
1400	935.623	1613.580	1026.897	821.356	456.199	1433.013	-53.465
1500	950.452	1678.649	1068.197	915.678	458.385	1502.719	-52.328
1600	963.253	1740.409	1108.297	1011.379	460.738	1572.263	-51.328
1700	974.359	1799.147	1147.222	1108.272	463.184	1641.633	-50.440
1800	984.042	1855.120	1185.007	1206.203	465.647	1710.923	-49.649
1900	992.524	1908.557	1221.693	1305.041	468.096	1780.022	-48.935
2000	999.985	1959.660	1257.323	1404.674	470.477	1849.021	-48.290
2100	1006.577	2008.612	1291.941	1505.009	472.712	1917.890	-47.704
2200	1012.425	2055.576	1325.592	1605.965	474.800	1986.658	-47.168
2300	1017.632	2100.697	1358.318	1707.473	476.736	2055.334	-46.677
2400	1022.285	2144.107	1390.160	1809.473	478.448	2123.880	-46.224
2500	1026.459	2185.925	1421.160	1911.914	479.949	2192.476	-45.808
2600	1030.214	2226.258	1451.354	2014.750	481.202	2260.897	-45.421
2700	1033.603	2265.203	1480.779	2117.944	482.212	2329.349	-45.063
2800	1036.672	2302.849	1509.471	2221.460	482.952	2397.790	-44.730
2900	1039.458	2339.277	1537.460	2325.269	483.393	2466.155	-44.419
3000	1041.995	2374.560	1564.778	2429.344	483.579	2534.537	-44.129
3100	1044.310	2408.765	1591.455	2533.661	483.432	2602.838	-43.857
3200	1046.428	2441.954	1617.517	2638.199	482.995	2671.225	-43.602
3300	1048.371	2474.185	1642.990	2742.940	482.248	2739.670	-43.364
3400	1050.156	2505.508	1667.900	2847.868	481.163	2808.054	-43.140
3500	1051.801	2535.974	1692.269	2952.967	479.746	2876.456	-42.928
3600	1053.319	2565.626	1716.119	3058.224	478.019	2944.993	-42.730
3700	1054.723	2594.505	1739.471	3163.627	475.950	3013.600	-42.544
3800	1056.024	2622.650	1762.343	3269.165	473.513	3082.205	-42.367
3900	1057.232	2650.097	1784.756	3374.829	470.748	3150.826	-42.200
4000	1058.355	2676.878	1806.725	3480.609	467.640	3219.666	-42.044
4100	1059.400	2703.024	1828.269	3586.497	464.153	3288.510	-41.895
4200	1060.375	2728.565	1849.402	3692.487	460.314	3357.436	-41.755
4300	1061.287	2753.527	1870.139	3798.570	456.110	3426.365	-41.621
4400	1062.139	2777.935	1890.494	3904.742	451.549	3495.490	-41.496
4500	1062.937	2801.814	1910.481	4010.996	446.648	3564.780	-41.378
4600	1063.686	2825.184	1930.113	4117.328	441.351	3634.192	-41.267
4700	1064.390	2848.068	1949.401	4223.732	435.675	3703.606	-41.160
4800	1065.051	2870.484	1968.358	4330.204	429.668	3773.253	-41.061
4900	1065.674	2892.451	1986.993	4436.741	423.252	3842.890	-40.965
5000	1066.261	2913.986	2005.319	4543.338	416.525	3912.854	-40.876

3.339. Tribenzo[*b,def,p*]chrysene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 66032-75-9
Point Group: C₁

Length: 15.86 Å
Width: 11.60 Å
Breadth: 5.044 Å
L/B Ratio: 1.367

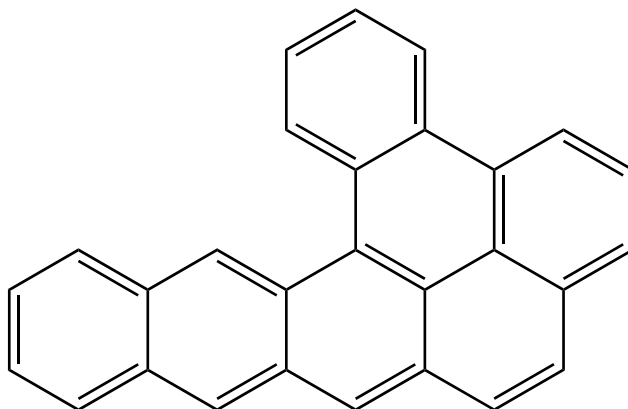
Cartesian coordinates:

C	5.2370	0.0984	-0.7662	C	0.5134	0.7547	0.1875	H	4.6211	3.3304	0.1190
C	5.4856	1.4629	-0.4771	C	1.2641	-1.5827	0.1681	H	3.8222	-1.4891	-0.8418
C	4.4564	2.2663	-0.0864	C	-0.0659	-2.0236	0.0211	H	2.2792	3.6802	0.5135
C	3.9900	-0.4306	-0.6007	C	-0.3551	-3.3978	0.0519	H	-0.0950	4.1224	0.6753
C	2.8913	0.3579	-0.1406	C	0.6347	-4.3292	0.3002	H	-2.4498	3.3355	0.4960
C	3.1349	1.7422	0.0504	C	1.9349	-3.8928	0.5526	H	-2.6801	-2.5335	-0.4325
C	2.0736	2.6168	0.3383	C	2.2377	-2.5448	0.4892	H	-1.3936	-3.7248	-0.1110
C	0.7723	2.1470	0.3456	C	-3.5239	-0.5353	-0.2563	H	0.3979	-5.3977	0.3201
C	-0.3261	3.0656	0.4982	C	-3.2573	0.8269	-0.0124	H	2.7162	-4.6183	0.8020
C	-1.6033	2.6379	0.4036	C	-4.3468	1.7384	0.0329	H	3.2685	-2.2282	0.6996
C	-1.9037	1.2514	0.1696	C	-5.6299	1.3057	-0.1645	H	-4.1301	2.7993	0.2301
C	-2.4568	-1.4659	-0.2759	C	-5.8923	-0.0603	-0.4173	H	-6.4659	2.0117	-0.1293
C	-0.8607	0.3225	0.1102	C	-4.8645	-0.9624	-0.4618	H	-6.9261	-0.3845	-0.5752
C	-1.1554	-1.0622	-0.0771	H	6.0605	-0.5251	-1.1299	H	-5.0574	-2.0237	-0.6548
C	1.5766	-0.1569	0.0676	H	6.5005	1.8580	-0.5869				

Table 3.339: Table of thermodynamic data as a function of temperature for Tribenzo[*b,def,p*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.976	480.559	480.559	∞
100	113.576	355.047	805.354	-45.031	507.020	554.763	-289.772
200	225.277	466.237	607.997	-28.352	493.019	608.090	-158.814
250	289.932	523.399	585.333	-15.484	486.431	637.620	-133.221
298.15	353.065	579.875	579.875	0.000	480.559	667.286	-116.903
300	355.463	582.067	579.882	0.655	480.342	668.443	-116.384
350	418.573	641.648	584.443	20.022	474.929	700.233	-104.502
400	477.160	701.423	595.332	42.437	470.232	732.739	-95.684
450	530.266	760.746	610.422	67.646	466.169	765.801	-88.890
500	577.750	819.121	628.383	95.369	462.652	799.308	-83.501
600	657.374	931.785	669.645	157.284	456.951	867.204	-75.495
700	720.317	1038.031	714.762	226.289	452.808	935.934	-69.839
800	770.771	1137.629	761.463	300.932	450.039	1005.146	-65.628
900	811.868	1230.865	808.496	380.132	448.467	1074.625	-62.368
1000	845.804	1318.215	855.148	463.068	447.927	1144.235	-59.767
1100	874.135	1400.197	901.010	549.106	448.221	1213.868	-57.641
1200	897.993	1477.309	945.854	637.746	449.209	1283.424	-55.865
1300	918.231	1550.008	989.558	728.584	450.707	1352.887	-54.359
1400	935.509	1618.705	1032.066	821.294	452.585	1422.224	-53.063
1500	950.343	1683.767	1073.364	915.605	454.760	1491.418	-51.935
1600	963.150	1745.519	1113.460	1011.295	457.102	1560.450	-50.942
1700	974.262	1804.251	1152.382	1108.178	459.537	1629.309	-50.062
1800	983.951	1860.219	1190.163	1206.100	461.991	1698.089	-49.276
1900	992.437	1913.651	1226.846	1304.929	464.432	1766.679	-48.568
2000	999.904	1964.750	1262.473	1404.554	466.805	1835.168	-47.929
2100	1006.501	2013.698	1297.089	1504.880	469.031	1903.528	-47.347
2200	1012.353	2060.659	1330.736	1605.829	471.112	1971.788	-46.815
2300	1017.564	2105.777	1363.459	1707.330	473.041	2039.956	-46.328
2400	1022.222	2149.184	1395.299	1809.323	474.746	2107.994	-45.878
2500	1026.399	2190.999	1426.296	1911.758	476.241	2176.083	-45.466
2600	1030.158	2231.330	1456.488	2014.589	477.488	2243.996	-45.081
2700	1033.550	2270.273	1485.911	2117.778	478.493	2311.940	-44.726
2800	1036.622	2307.917	1514.600	2221.289	479.228	2379.875	-44.396
2900	1039.411	2344.343	1542.587	2325.092	479.663	2447.733	-44.088
3000	1041.950	2379.624	1569.904	2429.162	479.845	2515.608	-43.800
3100	1044.267	2413.828	1596.578	2533.475	479.694	2583.403	-43.529
3200	1046.388	2447.016	1622.638	2638.009	479.252	2651.284	-43.277
3300	1048.332	2479.245	1648.110	2742.747	478.502	2719.223	-43.041
3400	1050.120	2510.568	1673.018	2847.671	477.414	2787.101	-42.818
3500	1051.767	2541.033	1697.385	2952.766	475.993	2854.997	-42.608
3600	1053.286	2570.683	1721.234	3058.020	474.263	2923.028	-42.411
3700	1054.692	2599.562	1744.584	3163.419	472.190	2991.129	-42.226
3800	1055.994	2627.706	1767.455	3268.955	469.750	3059.229	-42.051
3900	1057.203	2655.152	1789.866	3374.615	466.982	3127.344	-41.885
4000	1058.327	2681.932	1811.834	3480.392	463.871	3195.678	-41.730
4100	1059.374	2708.078	1833.376	3586.278	460.381	3264.018	-41.583
4200	1060.350	2733.618	1854.508	3692.265	456.540	3332.438	-41.444
4300	1061.263	2758.580	1875.243	3798.346	452.333	3400.861	-41.311
4400	1062.116	2782.988	1895.598	3904.515	447.770	3469.481	-41.187
4500	1062.915	2806.865	1915.584	4010.767	442.866	3538.266	-41.070
4600	1063.665	2830.235	1935.214	4117.097	437.568	3607.173	-40.960
4700	1064.369	2853.118	1954.502	4223.499	431.890	3676.082	-40.854
4800	1065.032	2875.534	1973.457	4329.969	425.880	3745.224	-40.755
4900	1065.655	2897.501	1992.092	4436.504	419.463	3814.356	-40.661
5000	1066.243	2919.036	2010.416	4543.099	412.734	3883.815	-40.573

3.340. Phenanthro[9,10,1-*gra*]naphthacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-54-3
Point Group: C₁

Length: 15.90 Å
Width: 11.60 Å
Breadth: 5.095 Å
L/B Ratio: 1.370

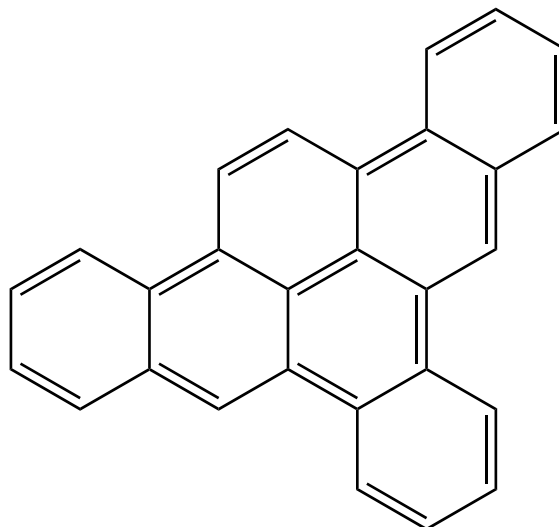
Cartesian coordinates:

C	5.8330	-1.0359	0.6129	C	-4.8168	1.5167	0.4320	H	5.6142	2.2579	-0.2959
C	6.2385	0.2894	0.2773	C	-5.2662	0.2170	0.6485	H	4.1970	-2.3944	0.8709
C	5.3150	1.2355	-0.0394	C	-4.3893	-0.8497	0.5467	H	3.2413	2.9036	-0.5258
C	4.5171	-1.3783	0.6137	C	-2.5629	0.6746	0.0680	H	1.8798	-1.7800	0.5075
C	3.5141	-0.4112	0.2747	C	-3.0372	-0.6392	0.2401	H	0.9468	3.5831	-0.6507
C	3.9184	0.9125	-0.0421	C	-0.2398	-0.1365	-0.1560	H	-1.3345	4.3617	-0.4968
C	2.9432	1.8681	-0.3182	C	-1.1560	0.9144	-0.1382	H	-3.7386	3.9123	-0.0781
C	2.1604	-0.7489	0.2475	C	-0.7604	-1.4958	-0.2382	H	-5.5185	2.3563	0.4935
C	1.1704	0.1818	-0.0916	C	-2.1223	-1.7434	0.0279	H	-6.3190	0.0382	0.8906
C	1.5845	1.5287	-0.3112	C	-2.6129	-3.0639	0.0143	H	-4.7474	-1.8801	0.6932
C	0.6100	2.5564	-0.4595	C	-1.7986	-4.1204	-0.3299	H	-3.6693	-3.2360	0.2721
C	-0.7205	2.2740	-0.3065	C	-0.4720	-3.8718	-0.6969	H	-2.1867	-5.1438	-0.3363
C	-1.6978	3.3433	-0.3159	C	0.0297	-2.5880	-0.6533	H	0.1660	-4.7001	-1.0223
C	-3.0020	3.1008	-0.0910	H	6.6034	-1.7705	0.8692	H	1.0718	-2.4200	-0.9579
C	-3.4746	1.7540	0.1407	H	7.3072	0.5275	0.2816				

Table 3.340: Table of thermodynamic data as a function of temperature for Phenanthro[9,10,1-*qra*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.732	484.503	484.503	∞
100	112.044	354.158	802.713	-44.855	511.139	558.970	-291.970
200	224.460	464.467	605.964	-28.299	497.015	612.440	-159.950
250	289.424	521.483	583.337	-15.463	490.395	642.062	-134.149
298.15	352.722	577.885	577.885	0.000	484.503	671.823	-117.698
300	355.124	580.075	577.892	0.655	484.285	672.983	-117.174
350	418.311	639.611	582.450	20.006	478.857	704.875	-105.195
400	476.929	699.353	593.330	42.409	474.148	737.483	-96.303
450	530.049	758.650	608.411	67.607	470.074	770.650	-89.453
500	577.543	817.002	626.362	95.320	466.547	804.261	-84.019
600	657.194	929.630	667.605	157.215	460.826	872.372	-75.945
700	720.175	1035.851	712.703	226.204	456.666	941.319	-70.241
800	770.671	1135.433	759.389	300.835	453.886	1010.749	-65.994
900	811.805	1228.660	806.408	380.027	452.305	1080.448	-62.706
1000	845.773	1316.005	853.047	462.958	451.761	1150.279	-60.083
1100	874.129	1397.986	898.899	548.995	452.053	1220.133	-57.938
1200	898.006	1475.098	943.735	637.635	453.042	1289.910	-56.147
1300	918.257	1547.798	987.432	728.475	454.542	1359.594	-54.628
1400	935.544	1616.497	1029.934	821.188	456.422	1429.152	-53.321
1500	950.385	1681.562	1071.227	915.503	458.601	1498.566	-52.184
1600	963.195	1743.317	1111.319	1011.197	460.948	1567.819	-51.183
1700	974.309	1802.052	1150.237	1108.085	463.388	1636.898	-50.295
1800	983.999	1858.022	1188.016	1206.012	465.846	1705.898	-49.503
1900	992.485	1911.457	1224.696	1304.845	468.292	1774.707	-48.789
2000	999.951	1962.558	1260.321	1404.475	470.669	1843.416	-48.144
2100	1006.547	2011.509	1294.935	1504.806	472.901	1911.995	-47.557
2200	1012.398	2058.471	1328.581	1605.759	474.986	1980.474	-47.021
2300	1017.608	2103.591	1361.303	1707.265	476.919	2048.860	-46.530
2400	1022.264	2147.001	1393.141	1809.262	478.629	2117.117	-46.077
2500	1026.439	2188.818	1424.137	1911.701	480.128	2185.424	-45.661
2600	1030.196	2229.150	1454.328	2014.536	481.379	2253.555	-45.274
2700	1033.587	2268.094	1483.751	2117.728	482.387	2321.718	-44.915
2800	1036.657	2305.740	1512.439	2221.243	483.126	2389.870	-44.583
2900	1039.445	2342.167	1540.425	2325.050	483.565	2457.946	-44.271
3000	1041.982	2377.449	1567.741	2429.124	483.750	2526.039	-43.981
3100	1044.298	2411.654	1594.415	2533.439	483.602	2594.051	-43.709
3200	1046.417	2444.843	1620.475	2637.977	483.163	2662.149	-43.454
3300	1048.361	2477.073	1645.947	2742.717	482.416	2730.306	-43.216
3400	1050.147	2508.397	1670.855	2847.644	481.330	2798.400	-42.991
3500	1051.792	2538.862	1695.221	2952.742	479.912	2866.513	-42.779
3600	1053.311	2568.513	1719.070	3057.998	478.184	2934.762	-42.581
3700	1054.716	2597.393	1742.420	3163.400	476.115	3003.080	-42.395
3800	1056.017	2625.537	1765.291	3268.938	473.676	3071.396	-42.218
3900	1057.225	2652.984	1787.702	3374.600	470.911	3139.729	-42.051
4000	1058.348	2679.765	1809.670	3480.380	467.802	3208.279	-41.895
4100	1059.394	2705.911	1831.212	3586.267	464.314	3276.836	-41.747
4200	1060.370	2731.452	1852.343	3692.256	460.475	3345.473	-41.606
4300	1061.281	2756.414	1873.079	3798.339	456.270	3414.113	-41.472
4400	1062.134	2780.822	1893.433	3904.510	451.709	3482.949	-41.347
4500	1062.932	2804.700	1913.419	4010.764	446.807	3551.951	-41.229
4600	1063.681	2828.070	1933.050	4117.095	441.510	3621.074	-41.118
4700	1064.385	2850.954	1952.337	4223.499	435.834	3690.199	-41.011
4800	1065.047	2873.370	1971.292	4329.971	429.825	3759.558	-40.911
4900	1065.670	2895.337	1989.927	4436.507	423.410	3828.906	-40.816
5000	1066.257	2916.872	2008.251	4543.104	416.682	3898.582	-40.727

3.341. Dibenzo[*h,rst*]pentaphene



Formula: $C_{28}H_{16}$
Mass: 352.427 g/mol
CAS Number: 192-47-2
Point Group: C_{2v}

Length: 15.90 Å
Width: 11.66 Å
Breadth: 3.891 Å
L/B Ratio: 1.363

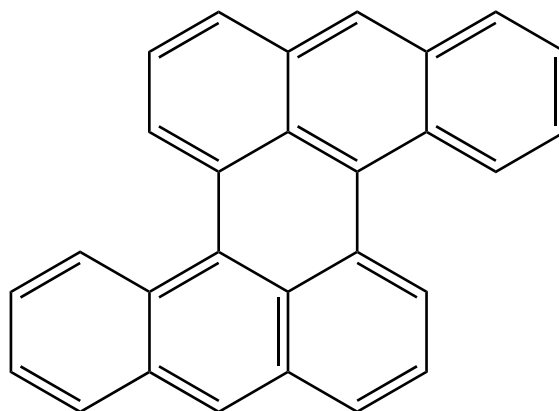
Cartesian coordinates:

C	4.9583	-2.6129	0.0000	C	-2.8100	1.0365	0.0000	H	5.4902	0.7566	0.0000
C	5.6515	-1.3864	0.0000	C	-0.7150	-0.1924	0.0000	H	3.0322	-3.5837	0.0000
C	4.9585	-0.2017	0.0000	C	-1.4145	-1.4068	0.0000	H	3.3775	1.9709	0.0000
C	3.5859	-2.6324	0.0000	C	-0.6874	-2.6297	0.0000	H	2.4951	3.5196	0.0000
C	2.8470	-1.4248	0.0000	C	0.6749	-2.6329	0.0000	H	1.2588	5.6764	0.0000
C	3.5419	-0.2022	0.0000	C	1.4078	-1.4135	0.0000	H	-1.2318	5.6823	0.0000
C	2.8149	1.0232	0.0000	C	0.7141	-0.1958	0.0000	H	-2.4783	3.5314	0.0000
C	1.4452	1.0423	0.0000	C	-2.8537	-1.4113	0.0000	H	-3.3681	1.9869	0.0000
C	-0.6970	2.3078	0.0000	C	-3.5428	-0.1854	0.0000	H	-1.2573	-3.5716	0.0000
C	0.7079	2.3045	0.0000	C	-4.9594	-0.1781	0.0000	H	1.2404	-3.5775	0.0000
C	1.3942	3.5274	0.0000	C	-5.6580	-1.3595	0.0000	H	-5.4865	0.7827	0.0000
C	0.7079	4.7303	0.0000	C	-4.9707	-2.5893	0.0000	H	-6.7529	-1.3569	0.0000
C	-0.6855	4.7336	0.0000	C	-3.5984	-2.6154	0.0000	H	-5.5420	-3.5234	0.0000
C	-1.3775	3.5339	0.0000	H	5.5251	-3.5497	0.0000	H	-3.0492	-3.5693	0.0000
C	-1.4402	1.0491	0.0000	H	6.7464	-1.3890	0.0000				

Table 3.341: Table of thermodynamic data as a function of temperature for Dibenzo[*h,rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-52.017	444.939	444.939	∞
100	114.555	353.216	802.545	-44.933	471.498	519.424	-271.314
200	224.641	464.558	605.766	-28.242	457.510	572.916	-149.627
250	288.769	521.518	583.194	-15.419	450.876	602.535	-125.890
298.15	351.573	577.759	577.759	0.000	444.939	632.297	-110.774
300	353.962	579.941	577.766	0.653	444.720	633.458	-110.293
350	416.883	639.276	582.308	19.939	439.226	665.361	-99.298
400	475.393	698.819	593.152	42.267	434.442	697.991	-91.146
450	528.497	757.933	608.183	67.387	430.291	731.189	-84.872
500	576.027	816.124	626.077	95.023	426.686	764.841	-79.901
600	655.813	928.486	667.198	156.773	420.820	833.053	-72.522
700	718.943	1034.506	712.176	225.631	416.530	902.124	-67.316
800	769.573	1133.932	758.749	300.146	413.634	971.697	-63.444
900	810.824	1227.037	805.665	379.234	411.949	1041.553	-60.449
1000	844.892	1314.284	852.211	462.072	411.312	1111.552	-58.060
1100	873.334	1396.184	897.979	548.025	411.521	1181.582	-56.107
1200	897.286	1473.230	942.739	636.590	412.433	1251.542	-54.477
1300	917.604	1545.876	986.367	727.362	413.865	1321.416	-53.094
1400	934.949	1614.529	1028.806	820.012	415.683	1391.168	-51.904
1500	949.842	1679.554	1070.041	914.270	417.805	1460.782	-50.868
1600	962.699	1741.276	1110.081	1009.912	420.100	1530.237	-49.956
1700	973.854	1799.982	1148.951	1106.753	422.492	1599.521	-49.146
1800	983.580	1855.927	1186.685	1204.636	424.907	1668.729	-48.424
1900	992.100	1909.340	1223.325	1303.429	427.312	1737.749	-47.773
2000	999.595	1960.423	1258.912	1403.021	429.653	1806.671	-47.184
2100	1006.217	2009.357	1293.491	1503.319	431.850	1875.464	-46.649
2200	1012.092	2056.304	1327.104	1604.240	433.903	1944.159	-46.159
2300	1017.323	2101.411	1359.796	1705.716	435.807	2012.762	-45.710
2400	1021.999	2144.809	1391.606	1807.686	437.489	2081.238	-45.296
2500	1026.192	2186.615	1422.575	1910.099	438.963	2149.765	-44.916
2600	1029.965	2226.938	1452.742	2012.910	440.190	2218.117	-44.562
2700	1033.370	2265.874	1482.141	2116.080	441.175	2286.501	-44.234
2800	1036.454	2303.512	1510.807	2219.574	441.893	2354.875	-43.930
2900	1039.253	2339.932	1538.773	2323.361	442.312	2423.175	-43.645
3000	1041.802	2375.208	1566.069	2427.416	442.479	2491.491	-43.380
3100	1044.128	2409.407	1592.725	2531.714	442.313	2559.728	-43.130
3200	1046.257	2442.591	1618.767	2636.235	441.858	2628.051	-42.898
3300	1048.209	2474.816	1644.222	2740.960	441.095	2696.433	-42.680
3400	1050.003	2506.135	1669.114	2845.872	439.995	2764.754	-42.474
3500	1051.656	2536.597	1693.466	2950.956	438.563	2833.093	-42.281
3600	1053.182	2566.244	1717.300	3056.198	436.822	2901.568	-42.100
3700	1054.593	2595.120	1740.637	3161.588	434.739	2970.113	-41.930
3800	1055.900	2623.262	1763.495	3267.114	432.289	3038.657	-41.768
3900	1057.113	2650.705	1785.893	3372.765	429.512	3107.217	-41.616
4000	1058.242	2677.483	1807.850	3478.533	426.393	3175.996	-41.473
4100	1059.292	2703.627	1829.380	3584.411	422.894	3244.780	-41.338
4200	1060.273	2729.165	1850.501	3690.390	419.045	3313.646	-41.210
4300	1061.188	2754.125	1871.226	3796.463	414.830	3382.515	-41.089
4400	1062.045	2778.531	1891.571	3902.625	410.260	3451.580	-40.975
4500	1062.847	2802.407	1911.547	4008.870	405.349	3520.811	-40.868
4600	1063.600	2825.776	1931.169	4115.193	400.044	3590.164	-40.767
4700	1064.307	2848.657	1950.447	4221.589	394.360	3659.518	-40.670
4800	1064.971	2871.072	1969.394	4328.053	388.344	3729.107	-40.580
4900	1065.597	2893.037	1988.021	4434.582	381.921	3798.685	-40.494
5000	1066.187	2914.571	2006.337	4541.171	375.186	3868.591	-40.414

3.342. Dibenzo[*a,j*]perylene



Other names: p-meso-Benzodianthrene

Formula: C₂₈H₁₆

Mass: 352.427 g/mol

CAS Number: 191-87-7

Point Group: S₂

Length: 16.03 Å

Width: 11.64 Å

Breadth: 4.712 Å

L/B Ratio: 1.377

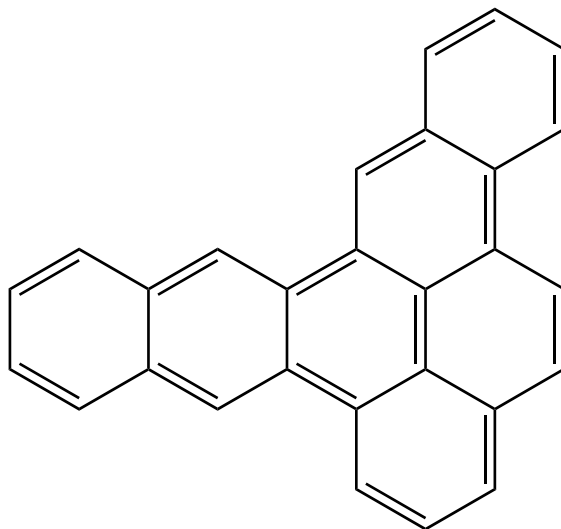
Cartesian coordinates:

C	4.8843	1.6598	-0.4060	C	-1.2355	3.5531	0.0236	H	5.7179	-1.5134	0.5178
C	5.6964	0.5581	-0.0224	C	0.0717	3.7244	0.3512	H	2.9273	2.4124	-0.7420
C	5.1134	-0.6375	0.2557	C	0.9379	2.6055	0.4212	H	3.7725	-2.9310	0.4725
C	3.5275	1.5534	-0.4121	C	-1.7577	2.2310	-0.1311	H	1.9124	-4.4053	0.0714
C	2.8564	0.3433	-0.0361	C	-0.8967	1.1002	-0.0539	H	-0.4791	-4.7169	-0.5742
C	3.6890	-0.7881	0.1946	C	-1.4469	-0.1992	-0.0573	H	-1.9777	-2.7976	-0.7331
C	3.1280	-2.0589	0.3049	C	-3.1311	2.0585	-0.2981	H	-1.9149	4.4062	-0.0824
C	1.7559	-2.2303	0.1273	C	-3.6909	0.7876	-0.1834	H	0.4798	4.7210	0.5493
C	1.2338	-3.5516	-0.0351	C	-2.8558	-0.3436	0.0393	H	1.9784	2.8022	0.7139
C	-0.0716	-3.7212	-0.3706	C	-3.5231	-1.5564	0.4127	H	-3.7771	2.9302	-0.4622
C	-0.9375	-2.6018	-0.4390	C	-4.8799	-1.6642	0.4150	H	-2.9211	-2.4182	0.7320
C	1.4468	0.2005	0.0528	C	-5.6956	-0.5611	0.0431	H	-5.3633	-2.6005	0.7132
C	0.8961	-1.0988	0.0478	C	-5.1155	0.6360	-0.2346	H	-6.7822	-0.6877	0.0075
C	-0.5188	-1.3293	-0.1290	H	5.3705	2.5936	-0.7076	H	-5.7226	1.5124	-0.4890
C	0.5188	1.3313	0.1186	H	6.7828	0.6843	0.0209				

Table 3.342: Table of thermodynamic data as a function of temperature for Dibenzo[*a,j*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-51.609	562.932	562.932	∞
100	111.010	344.977	793.757	-44.878	589.546	638.296	-333.405
200	224.683	455.051	596.794	-28.349	575.396	692.704	-180.912
250	289.937	512.149	574.125	-15.494	568.794	722.795	-151.017
298.15	353.472	568.663	568.663	0.000	562.932	753.002	-131.920
300	355.883	570.856	568.669	0.656	562.717	754.180	-131.312
350	419.268	630.525	573.237	20.051	557.331	786.529	-117.381
400	478.025	690.405	584.142	42.505	552.674	819.588	-107.025
450	531.222	749.836	599.257	67.760	548.657	853.199	-99.035
500	578.740	808.314	617.249	95.532	545.189	887.248	-92.688
600	658.333	921.156	658.580	157.545	539.586	956.216	-83.244
700	721.184	1027.544	703.770	226.642	535.534	1026.002	-76.560
800	771.530	1127.251	750.542	301.367	532.847	1096.256	-71.577
900	812.523	1220.570	797.640	380.637	531.345	1166.769	-67.716
1000	846.368	1307.985	844.351	463.634	530.866	1237.405	-64.634
1100	874.620	1390.017	890.267	549.725	531.213	1308.059	-62.113
1200	898.412	1467.168	935.160	638.409	532.246	1378.630	-60.009
1300	918.595	1539.898	978.908	729.287	533.783	1449.106	-58.225
1400	935.826	1608.620	1021.456	822.030	535.695	1519.452	-56.690
1500	950.623	1673.703	1062.789	916.371	537.900	1589.654	-55.356
1600	963.397	1735.472	1102.917	1012.088	540.268	1659.692	-54.182
1700	974.482	1794.218	1141.868	1108.994	542.727	1729.554	-53.142
1800	984.147	1850.198	1179.677	1206.937	545.201	1799.337	-52.214
1900	992.614	1903.640	1216.385	1305.784	547.660	1868.929	-51.379
2000	1000.063	1954.747	1252.035	1405.425	550.050	1938.419	-50.625
2100	1006.645	2003.703	1286.671	1505.767	552.292	2007.778	-49.940
2200	1012.485	2050.670	1320.338	1606.730	554.386	2077.037	-49.314
2300	1017.684	2095.793	1353.079	1708.243	556.328	2146.204	-48.741
2400	1022.332	2139.206	1384.936	1810.248	558.045	2215.241	-48.212
2500	1026.500	2181.025	1415.948	1912.694	559.550	2284.327	-47.727
2600	1030.251	2221.360	1446.154	2015.534	560.807	2353.237	-47.276
2700	1033.637	2260.306	1475.591	2118.732	561.820	2422.179	-46.859
2800	1036.703	2297.954	1504.292	2222.251	562.564	2491.109	-46.471
2900	1039.486	2334.382	1532.292	2326.063	563.007	2559.964	-46.109
3000	1042.020	2369.666	1559.619	2430.140	563.196	2628.835	-45.771
3100	1044.333	2403.872	1586.304	2534.459	563.052	2697.626	-45.454
3200	1046.449	2437.062	1612.374	2639.000	562.616	2766.502	-45.158
3300	1048.390	2469.293	1637.856	2743.743	561.872	2835.437	-44.880
3400	1050.174	2500.617	1662.772	2848.673	560.789	2904.310	-44.618
3500	1051.818	2531.083	1687.148	2953.774	559.374	2973.200	-44.372
3600	1053.335	2560.735	1711.004	3059.032	557.649	3042.226	-44.141
3700	1054.738	2589.615	1734.362	3164.437	555.581	3111.322	-43.923
3800	1056.038	2617.761	1757.241	3269.976	553.145	3180.417	-43.717
3900	1057.244	2645.208	1779.659	3375.641	550.382	3249.527	-43.522
4000	1058.366	2671.989	1801.633	3481.422	547.275	3318.855	-43.339
4100	1059.411	2698.136	1823.182	3587.312	543.788	3388.189	-43.165
4200	1060.386	2723.677	1844.319	3693.302	539.951	3457.603	-43.001
4300	1061.296	2748.639	1865.061	3799.387	535.747	3527.021	-42.844
4400	1062.148	2773.048	1885.420	3905.560	531.188	3596.635	-42.697
4500	1062.946	2796.926	1905.412	4011.815	526.287	3666.414	-42.558
4600	1063.694	2820.297	1925.047	4118.147	520.991	3736.314	-42.426
4700	1064.397	2843.180	1944.340	4224.552	515.316	3806.217	-42.300
4800	1065.059	2865.597	1963.300	4331.025	509.310	3876.353	-42.182
4900	1065.681	2887.564	1981.939	4437.562	502.895	3946.478	-42.069
5000	1066.268	2909.099	2000.267	4544.160	496.169	4016.931	-41.964

3.343. Naphtho[2,1,8-*fgh*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 19301-88-3
Point Group: C_s

Length: 15.90 Å
Width: 11.65 Å
Breadth: 3.887 Å
L/B Ratio: 1.365

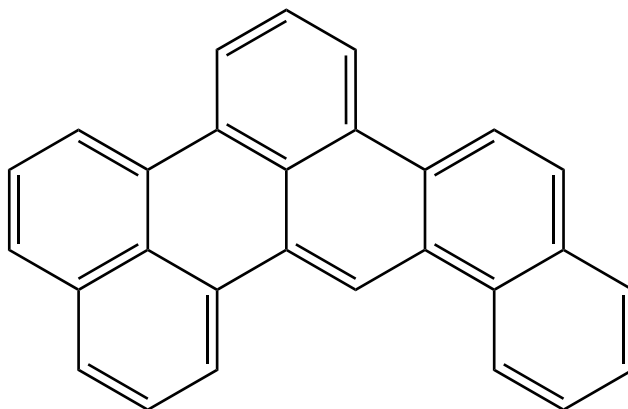
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C	5.4593	-2.4391	0.0000	C	-0.9361	4.2652	0.0000	H	5.6703	0.9729	0.0000
C	6.0322	-1.1435	0.0000	C	-1.2724	0.5295	0.0000	H	3.6503	-3.5956	0.0000
C	5.2353	-0.0327	0.0000	C	-0.6810	1.8368	0.0000	H	3.4145	1.9683	0.0000
C	4.1014	-2.5970	0.0000	C	-1.5102	2.9759	0.0000	H	1.3976	-2.5979	0.0000
C	3.2482	-1.4579	0.0000	C	-2.9315	2.8118	0.0000	H	-0.3800	-2.7820	0.0000
C	3.8186	-0.1682	0.0000	C	-3.4824	1.5714	0.0000	H	2.3561	3.4103	0.0000
C	2.9680	0.9607	0.0000	C	-2.6640	0.3977	0.0000	H	0.8829	5.4082	0.0000
C	1.8407	-1.5888	0.0000	C	-2.4295	-2.0430	0.0000	H	-1.5912	5.1437	0.0000
C	1.0161	-0.4813	0.0000	C	-3.2621	-0.9084	0.0000	H	-3.5618	3.7084	0.0000
C	1.5942	0.8239	0.0000	C	-4.6676	-1.0908	0.0000	H	-4.5747	1.4337	0.0000
C	-0.4384	-0.6375	0.0000	C	-5.2097	-2.3503	0.0000	H	-5.3098	-0.1968	0.0000
C	-1.0162	-1.8820	0.0000	C	-4.3726	-3.4853	0.0000	H	-6.2962	-2.4860	0.0000
C	0.7295	2.0020	0.0000	C	-3.0094	-3.3373	0.0000	H	-4.8234	-4.4831	0.0000
C	1.2627	3.2817	0.0000	H	6.1212	-3.3113	0.0000	H	-2.3518	-4.2139	0.0000
C	0.4320	4.4104	0.0000	H	7.1228	-1.0462	0.0000				

Table 3.343: Table of thermodynamic data as a function of temperature for Naphtho[2,1,8-*fgh*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-52.148	445.534	445.534	∞
100	114.446	366.000	815.349	-44.935	472.091	518.738	-270.956
200	224.665	477.265	618.534	-28.254	458.092	570.958	-149.116
250	288.911	534.244	595.951	-15.427	451.463	599.940	-125.348
298.15	351.743	590.514	590.514	0.000	445.534	629.089	-110.211
300	354.131	592.697	590.521	0.653	445.315	630.226	-109.730
350	417.023	652.056	595.065	19.947	439.829	661.491	-98.720
400	475.484	711.615	605.913	42.281	435.051	693.482	-90.558
450	528.541	770.737	620.948	67.405	430.903	726.039	-84.275
500	576.034	828.930	638.846	95.042	427.300	759.051	-79.296
600	655.782	941.290	679.973	156.790	421.432	825.982	-71.907
700	718.911	1047.305	724.955	225.645	417.139	893.774	-66.693
800	769.555	1146.727	771.530	300.158	414.240	962.067	-62.815
900	810.825	1239.831	818.448	379.244	412.555	1030.643	-59.816
1000	844.911	1327.079	864.995	462.084	411.918	1099.363	-57.424
1100	873.368	1408.982	910.764	548.040	412.130	1168.113	-55.468
1200	897.332	1486.032	955.525	636.608	413.046	1236.794	-53.835
1300	917.657	1558.681	999.154	727.385	414.483	1305.387	-52.450
1400	935.007	1627.338	1041.595	820.041	416.307	1373.859	-51.258
1500	949.903	1692.368	1082.831	914.305	418.435	1442.191	-50.221
1600	962.760	1754.094	1122.873	1009.953	420.735	1510.365	-49.307
1700	973.915	1812.803	1161.744	1106.800	423.134	1578.367	-48.496
1800	983.640	1868.752	1199.481	1204.689	425.555	1646.293	-47.773
1900	992.158	1922.168	1236.122	1303.488	427.966	1714.030	-47.121
2000	999.652	1973.254	1271.711	1403.086	430.312	1781.669	-46.531
2100	1006.272	2022.190	1306.291	1503.389	432.515	1849.179	-45.995
2200	1012.144	2069.140	1339.906	1604.316	434.574	1916.590	-45.505
2300	1017.373	2114.249	1372.599	1705.797	436.483	1983.910	-45.055
2400	1022.047	2157.649	1404.411	1807.772	438.170	2051.102	-44.640
2500	1026.237	2199.457	1435.382	1910.190	439.648	2118.344	-44.259
2600	1030.008	2239.782	1465.549	2013.005	440.879	2185.412	-43.905
2700	1033.412	2278.720	1494.950	2116.179	441.869	2252.512	-43.577
2800	1036.493	2316.359	1523.617	2219.677	442.591	2319.602	-43.272
2900	1039.291	2352.781	1551.585	2323.468	443.014	2386.616	-42.987
3000	1041.838	2388.058	1578.882	2427.527	443.185	2453.648	-42.721
3100	1044.162	2422.258	1605.539	2531.829	443.023	2520.599	-42.471
3200	1046.289	2455.443	1631.583	2636.353	442.571	2587.637	-42.238
3300	1048.240	2487.669	1657.039	2741.080	441.811	2654.734	-42.020
3400	1050.033	2518.989	1681.932	2845.995	440.713	2721.769	-41.814
3500	1051.684	2549.451	1706.285	2951.082	439.284	2788.823	-41.620
3600	1053.209	2579.100	1730.120	3056.328	437.546	2856.013	-41.439
3700	1054.619	2607.976	1753.457	3161.720	435.466	2923.272	-41.268
3800	1055.925	2636.118	1776.316	3267.248	433.018	2990.531	-41.107
3900	1057.137	2663.562	1798.716	3372.902	430.244	3057.805	-40.954
4000	1058.265	2690.341	1820.673	3478.673	427.127	3125.298	-40.811
4100	1059.314	2716.486	1842.205	3584.552	423.631	3192.797	-40.676
4200	1060.294	2742.024	1863.326	3690.533	419.783	3260.376	-40.548
4300	1061.208	2766.984	1884.052	3796.609	415.571	3327.959	-40.426
4400	1062.064	2791.391	1904.397	3902.773	411.003	3395.739	-40.312
4500	1062.866	2815.268	1924.374	4009.020	406.094	3463.683	-40.205
4600	1063.618	2838.637	1943.997	4115.345	400.791	3531.750	-40.103
4700	1064.324	2861.519	1963.276	4221.742	395.108	3599.819	-40.007
4800	1064.988	2883.933	1982.223	4328.208	389.094	3668.121	-39.916
4900	1065.613	2905.899	2000.851	4434.738	382.672	3736.413	-39.830
5000	1066.203	2927.433	2019.168	4541.329	375.939	3805.032	-39.750

3.344. Naphtho[1,2-*b*]perylene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-41-8
Point Group: C_s

Length: 15.91 Å
Width: 11.65 Å
Breadth: 3.887 Å
L/B Ratio: 1.365

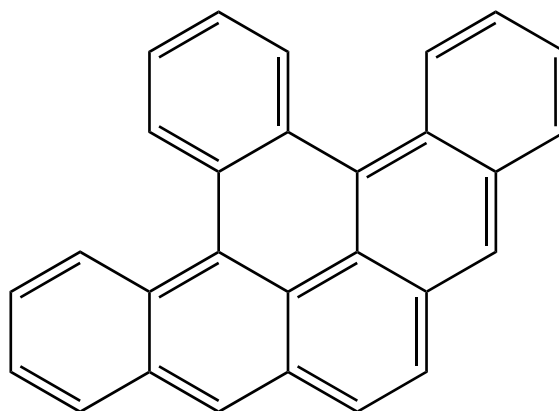
Cartesian coordinates:

C	4.8038	-2.5408	0.0000	C	-0.4237	-0.3860	0.0000	H	6.6031	0.3569	0.0000
C	5.9189	-1.6807	0.0000	C	-0.6170	1.0368	0.0000	H	2.6520	-2.6865	0.0000
C	5.7406	-0.3192	0.0000	C	-1.9240	1.5974	0.0000	H	5.1225	2.2977	0.0000
C	3.5315	-2.0247	0.0000	C	-3.0905	0.7154	0.0000	H	2.8305	3.2610	0.0000
C	3.3200	-0.6252	0.0000	C	-4.3730	1.2245	0.0000	H	0.9997	-1.9953	0.0000
C	4.4366	0.2306	0.0000	C	-5.4931	0.3699	0.0000	H	1.1906	3.9468	0.0000
C	4.2405	1.6471	0.0000	C	-5.3275	-0.9894	0.0000	H	-1.1075	4.9047	0.0000
C	2.9875	2.1715	0.0000	C	-1.5898	-1.2680	0.0000	H	-3.0912	3.4032	0.0000
C	1.9947	-0.0578	0.0000	C	-2.8974	-0.6978	0.0000	H	-4.5222	2.3154	0.0000
C	1.8323	1.3286	0.0000	C	-4.0228	-1.5496	0.0000	H	-6.4963	0.8086	0.0000
C	0.8462	-0.8988	0.0000	C	-3.8380	-2.9578	0.0000	H	-6.1934	-1.6610	0.0000
C	0.5054	1.8896	0.0000	C	-2.5752	-3.4866	0.0000	H	-4.7198	-3.6085	0.0000
C	0.3073	3.2903	0.0000	C	-1.4482	-2.6406	0.0000	H	-2.4253	-4.5713	0.0000
C	-0.9599	3.8198	0.0000	H	4.9613	-3.6242	0.0000	H	-0.4387	-3.0801	0.0000
C	-2.0778	2.9730	0.0000	H	6.9267	-2.1085	0.0000				

Table 3.344: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*b*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-52.253	461.280	461.280	∞
100	114.976	365.358	815.760	-45.040	487.732	534.443	-279.159
200	225.194	476.967	618.514	-28.309	473.783	586.708	-153.229
250	289.478	534.069	595.888	-15.455	467.181	615.702	-128.641
298.15	352.341	590.441	590.441	0.000	461.280	644.857	-112.974
300	354.730	592.628	590.448	0.654	461.062	645.994	-112.475
350	417.648	652.081	595.000	19.979	455.607	677.260	-101.073
400	476.122	711.724	605.864	42.344	450.860	709.247	-92.616
450	529.176	770.922	620.922	67.500	446.744	741.798	-86.104
500	576.650	829.181	638.844	95.169	443.173	774.798	-80.941
600	656.326	941.647	680.022	156.975	437.363	841.699	-73.275
700	719.360	1047.739	725.054	225.879	433.120	909.451	-67.863
800	769.909	1147.215	771.675	300.432	430.260	977.698	-63.836
900	811.095	1240.355	818.633	379.550	428.606	1046.223	-60.720
1000	845.111	1327.628	865.215	462.413	427.993	1114.889	-58.235
1100	873.513	1409.548	911.015	548.386	428.222	1183.583	-56.203
1200	897.433	1486.608	955.803	636.967	429.151	1252.207	-54.506
1300	917.726	1559.264	999.455	727.752	430.596	1320.742	-53.067
1400	935.051	1627.926	1041.916	820.413	432.425	1389.155	-51.829
1500	949.927	1692.957	1083.171	914.680	434.557	1457.428	-50.751
1600	962.771	1754.684	1123.228	1010.331	436.859	1525.543	-49.803
1700	973.916	1813.394	1162.113	1107.178	439.258	1593.486	-48.961
1800	983.634	1869.343	1199.862	1205.066	441.679	1661.353	-48.210
1900	992.146	1922.758	1236.514	1303.865	444.089	1729.031	-47.533
2000	999.636	1973.843	1272.112	1403.461	446.434	1796.611	-46.922
2100	1006.253	2022.779	1306.702	1503.763	448.635	1864.062	-46.365
2200	1012.124	2069.728	1340.325	1604.687	450.691	1931.414	-45.857
2300	1017.351	2114.836	1373.025	1706.166	452.598	1998.676	-45.390
2400	1022.024	2158.235	1404.844	1808.139	454.283	2065.809	-44.960
2500	1026.214	2200.042	1435.821	1910.555	455.759	2132.993	-44.566
2600	1029.985	2240.366	1465.994	2013.368	456.988	2200.002	-44.198
2700	1033.389	2279.303	1495.399	2116.539	457.976	2267.043	-43.858
2800	1036.471	2316.941	1524.072	2220.035	458.695	2334.075	-43.542
2900	1039.269	2353.362	1552.044	2323.824	459.116	2401.031	-43.246
3000	1041.816	2388.639	1579.345	2427.880	459.285	2468.005	-42.971
3100	1044.141	2422.838	1606.006	2532.180	459.120	2534.898	-42.712
3200	1046.269	2456.022	1632.053	2636.702	458.666	2601.878	-42.470
3300	1048.220	2488.248	1657.512	2741.428	457.904	2668.917	-42.245
3400	1050.014	2519.567	1682.408	2846.341	456.805	2735.895	-42.031
3500	1051.666	2550.029	1706.764	2951.426	455.374	2802.891	-41.830
3600	1053.191	2579.677	1730.602	3056.670	453.634	2870.022	-41.642
3700	1054.601	2608.553	1753.942	3162.060	451.552	2937.224	-41.465
3800	1055.908	2636.695	1776.804	3267.586	449.103	3004.425	-41.298
3900	1057.121	2664.138	1799.205	3373.239	446.327	3071.642	-41.139
4000	1058.249	2690.917	1821.165	3479.008	443.208	3139.077	-40.991
4100	1059.299	2717.061	1842.698	3584.886	439.710	3206.518	-40.851
4200	1060.279	2742.599	1863.822	3690.865	435.861	3274.040	-40.718
4300	1061.194	2767.559	1884.550	3796.939	431.648	3341.566	-40.591
4400	1062.050	2791.965	1904.896	3903.102	427.078	3409.288	-40.473
4500	1062.852	2815.841	1924.875	4009.348	422.168	3477.175	-40.361
4600	1063.605	2839.210	1944.499	4115.671	416.863	3545.185	-40.256
4700	1064.311	2862.092	1963.780	4222.067	411.179	3613.196	-40.155
4800	1064.976	2884.506	1982.729	4328.532	405.164	3681.441	-40.061
4900	1065.602	2906.472	2001.357	4435.061	398.741	3749.676	-39.971
5000	1066.192	2928.006	2019.676	4541.651	392.007	3818.238	-39.888

3.345. Naphtho[1,2,3,4-*rst*]pentaphene



Other names: homeo-Cerodianthrene
Tribenzo[*a,i,l*]pyrene

Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 191-20-8
Point Group: C₂

Length: 16.01 Å
Width: 11.66 Å
Breadth: 4.765 Å
L/B Ratio: 1.374

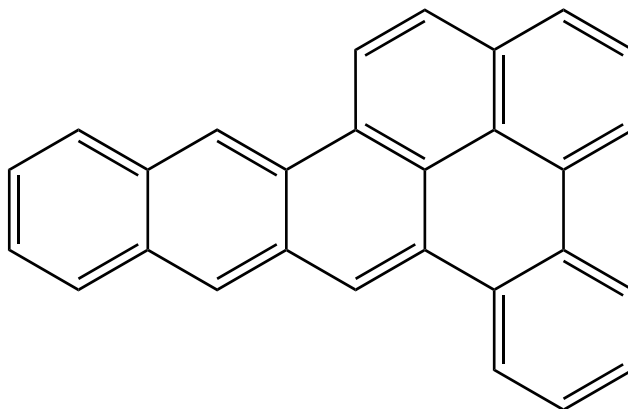
Cartesian coordinates:

C	5.0765	1.1976	-0.3559	C	0.7231	-0.9594	0.0487	H	5.4288	-2.1093	0.3610
C	5.7150	-0.0270	-0.0686	C	0.6908	1.4779	0.1332	H	3.2482	2.2574	-0.5836
C	4.9559	-1.1388	0.1713	C	-0.6973	1.4748	-0.1327	H	3.3021	-3.2075	0.3877
C	3.7106	1.2942	-0.3293	C	-1.3048	2.7093	-0.4555	H	1.2431	-4.3930	0.1482
C	2.8837	0.1820	-0.0081	C	-0.6532	3.9073	-0.2728	H	-1.2238	-4.3991	-0.1220
C	3.5365	-1.0599	0.1611	C	0.6367	3.9103	0.2718	H	-3.2864	-3.2237	-0.3807
C	2.7794	-2.2514	0.2570	C	1.2934	2.7151	0.4550	H	-2.3247	2.7196	-0.8633
C	1.4130	-2.2132	0.1305	C	-2.8847	0.1689	0.0061	H	-1.1431	4.8523	-0.5284
C	0.6751	-3.4578	0.0804	C	-3.5311	-1.0764	-0.1628	H	1.1224	4.8575	0.5269
C	-0.6596	-3.4610	-0.0612	C	-4.9502	-1.1618	-0.1788	H	2.3133	2.7296	0.8628
C	-1.4028	-2.2200	-0.1202	C	-5.7153	-0.0532	0.0562	H	-5.4178	-2.1347	-0.3693
C	-2.7684	-2.2648	-0.2518	C	-5.0835	1.1746	0.3448	H	-6.8084	-0.1094	0.0441
C	-0.7187	-0.9627	-0.0421	C	-3.7180	1.2774	0.3233	H	-5.6986	2.0457	0.5941
C	-1.4467	0.2325	-0.0753	H	5.6867	2.0713	-0.6081	H	-3.2611	2.2430	0.5787
C	1.4457	0.2390	0.0770	H	6.8083	-0.0785	-0.0613				

Table 3.345: Table of thermodynamic data as a function of temperature for Naphtho[1,2,3,4-*rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.586	515.093	515.093	∞
100	111.374	344.945	793.238	-44.829	541.756	590.509	-308.444
200	224.365	455.053	596.548	-28.299	527.606	644.914	-168.431
250	289.415	512.056	573.919	-15.466	520.983	675.007	-141.032
298.15	352.839	568.467	568.467	0.000	515.093	705.221	-123.549
300	355.247	570.657	568.474	0.655	514.876	706.400	-122.993
350	418.577	630.223	573.033	20.016	509.458	738.761	-110.252
400	477.316	690.009	583.920	42.436	504.765	771.838	-100.790
450	530.520	749.357	599.012	67.655	500.713	805.470	-93.495
500	578.060	807.762	616.976	95.393	497.210	839.545	-87.705
600	657.718	920.485	658.251	157.341	491.542	908.575	-79.097
700	720.645	1026.784	703.385	226.379	487.433	978.432	-73.010
800	771.063	1126.424	750.106	301.054	484.696	1048.766	-68.476
900	812.119	1219.692	797.157	380.281	483.150	1119.364	-64.965
1000	846.019	1307.067	843.827	463.240	482.634	1190.091	-62.163
1100	874.317	1389.068	889.705	549.298	482.948	1260.837	-59.871
1200	898.148	1466.194	934.565	637.955	483.952	1331.505	-57.958
1300	918.364	1538.904	978.283	728.808	485.465	1402.079	-56.335
1400	935.622	1607.610	1020.804	821.529	487.355	1472.526	-54.939
1500	950.441	1672.680	1062.112	915.851	489.540	1542.829	-53.725
1600	963.235	1734.438	1102.219	1011.550	491.891	1612.970	-52.657
1700	974.336	1793.175	1141.150	1108.442	494.335	1682.936	-51.709
1800	984.016	1849.146	1178.941	1206.370	496.795	1752.824	-50.865
1900	992.495	1902.582	1215.632	1305.205	499.242	1822.521	-50.104
2000	999.955	1953.684	1251.266	1404.835	501.621	1892.117	-49.416
2100	1006.547	2002.634	1285.888	1505.167	503.852	1961.583	-48.791
2200	1012.394	2049.597	1319.542	1606.120	505.937	2030.949	-48.220
2300	1017.602	2094.716	1352.271	1707.625	507.870	2100.223	-47.697
2400	1022.256	2138.125	1384.116	1809.622	509.579	2169.368	-47.214
2500	1026.430	2179.942	1415.118	1912.060	511.077	2238.562	-46.771
2600	1030.186	2220.274	1445.315	2014.894	512.327	2307.581	-46.359
2700	1033.576	2259.218	1474.742	2118.085	513.334	2376.631	-45.978
2800	1036.646	2296.863	1503.435	2221.598	514.072	2445.671	-45.624
2900	1039.433	2333.290	1531.426	2325.404	514.510	2514.635	-45.293
3000	1041.970	2368.572	1558.746	2429.477	514.694	2583.615	-44.984
3100	1044.286	2402.776	1585.424	2533.791	514.544	2652.516	-44.694
3200	1046.405	2435.965	1611.487	2638.327	514.105	2721.501	-44.423
3300	1048.349	2468.194	1636.962	2743.066	513.356	2790.546	-44.170
3400	1050.135	2499.518	1661.873	2847.992	512.269	2859.529	-43.930
3500	1051.781	2529.982	1686.243	2953.089	510.850	2928.529	-43.705
3600	1053.300	2559.634	1710.094	3058.344	509.121	2997.666	-43.494
3700	1054.705	2588.512	1733.446	3163.745	507.050	3066.872	-43.296
3800	1056.007	2616.657	1756.320	3269.281	504.611	3136.076	-43.107
3900	1057.215	2644.103	1778.733	3374.943	501.844	3205.297	-42.929
4000	1058.338	2670.884	1800.703	3480.721	498.735	3274.736	-42.763
4100	1059.384	2697.030	1822.247	3586.608	495.245	3344.180	-42.604
4200	1060.360	2722.570	1843.381	3692.596	491.405	3413.705	-42.455
4300	1061.272	2747.532	1864.118	3798.678	487.199	3483.233	-42.312
4400	1062.125	2771.940	1884.474	3904.848	482.638	3552.958	-42.178
4500	1062.924	2795.818	1904.462	4011.101	477.735	3622.848	-42.052
4600	1063.673	2819.188	1924.094	4117.431	472.437	3692.859	-41.933
4700	1064.377	2842.071	1943.383	4223.834	466.760	3762.873	-41.819
4800	1065.039	2864.487	1962.340	4330.305	460.751	3833.120	-41.712
4900	1065.662	2886.454	1980.976	4436.841	454.334	3903.356	-41.609
5000	1066.250	2907.989	1999.302	4543.437	447.606	3973.920	-41.514

3.346. Benzo[*a*]naphtho[8,1,2-*cde*]naphthacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 192-70-1
Point Group: C_s

Length: 16.04 Å
Width: 11.39 Å
Breadth: 3.886 Å
L/B Ratio: 1.408

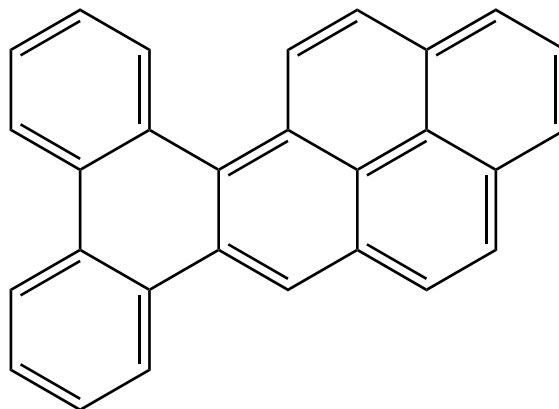
Cartesian coordinates:

C	-6.4906	0.5086	0.0000	C	3.3240	3.2889	0.0000	H	-5.3050	-2.7016	0.0000
C	-6.4891	-0.9151	0.0000	C	2.0780	1.1881	0.0000	H	-5.3102	2.2975	0.0000
C	-5.3162	-1.6058	0.0000	C	2.0921	2.5978	0.0000	H	-2.8454	-2.6960	0.0000
C	-5.3189	1.2017	0.0000	C	0.8547	3.3110	0.0000	H	-2.8464	2.3036	0.0000
C	-4.0667	0.5088	0.0000	C	-0.3278	2.6403	0.0000	H	-0.4120	-2.7100	0.0000
C	-4.0652	-0.9102	0.0000	C	-0.3679	1.2129	0.0000	H	5.4547	0.6365	0.0000
C	-2.8468	-1.5989	0.0000	C	0.8260	0.4927	0.0000	H	5.4650	3.1198	0.0000
C	-2.8506	1.2018	0.0000	C	3.2939	-0.9811	0.0000	H	3.3228	4.3848	0.0000
C	-1.6359	0.5186	0.0000	C	2.0725	-1.6764	0.0000	H	0.8801	4.4067	0.0000
C	-1.6379	-0.9032	0.0000	C	2.0859	-3.0789	0.0000	H	-1.2867	3.1814	0.0000
C	-0.3921	-1.6079	0.0000	C	3.2798	-3.7801	0.0000	H	1.1265	-3.6190	0.0000
C	0.8045	-0.9489	0.0000	C	4.4908	-3.0897	0.0000	H	3.2732	-4.8749	0.0000
C	3.3101	0.4789	0.0000	C	4.4949	-1.7052	0.0000	H	5.4364	-3.6415	0.0000
C	4.5010	1.1863	0.0000	H	-7.4515	1.0334	0.0000	H	5.4471	-1.1525	0.0000
C	4.5074	2.5888	0.0000	H	-7.4490	-1.4418	0.0000				

Table 3.346: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[8,1,2-*cde*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.854	453.474	453.474	∞
100	113.251	357.800	806.366	-44.857	480.109	527.576	-275.572
200	224.355	468.509	609.762	-28.251	466.035	580.652	-151.648
250	288.900	525.454	587.178	-15.431	459.399	610.073	-127.465
298.15	351.908	581.738	581.738	0.000	453.474	639.645	-112.061
300	354.302	583.922	581.745	0.653	453.255	640.799	-111.571
350	417.294	643.316	586.292	19.958	447.780	672.501	-100.363
400	475.803	702.914	597.146	42.307	443.017	704.928	-92.052
450	528.877	762.075	612.191	67.448	438.885	737.920	-85.654
500	576.369	820.304	630.101	95.102	435.299	771.363	-80.582
600	656.091	932.723	671.252	156.883	429.464	839.154	-73.053
700	719.183	1038.783	716.260	225.766	425.200	907.800	-67.739
800	769.793	1138.239	762.859	300.304	422.326	976.944	-63.787
900	811.032	1231.369	809.798	379.413	420.663	1046.368	-60.728
1000	845.092	1318.638	856.366	462.272	420.046	1115.932	-58.289
1100	873.527	1400.557	902.153	548.245	420.274	1185.526	-56.295
1200	897.472	1477.619	946.929	636.828	421.206	1255.048	-54.630
1300	917.782	1550.279	990.573	727.618	422.656	1324.482	-53.217
1400	935.118	1618.945	1033.027	820.286	424.491	1393.793	-52.002
1500	950.002	1683.982	1074.275	914.560	426.630	1462.965	-50.944
1600	962.850	1745.714	1114.328	1010.218	428.940	1531.977	-50.013
1700	973.996	1804.429	1153.209	1107.074	431.347	1600.817	-49.186
1800	983.714	1860.382	1190.954	1204.970	433.776	1669.580	-48.449
1900	992.226	1913.802	1227.604	1303.776	436.194	1738.154	-47.784
2000	999.713	1964.891	1263.200	1403.381	438.547	1806.629	-47.183
2100	1006.329	2013.830	1297.788	1503.690	440.756	1874.975	-46.636
2200	1012.197	2060.783	1331.409	1604.622	442.820	1943.222	-46.137
2300	1017.422	2105.894	1364.108	1706.108	444.733	2011.378	-45.679
2400	1022.091	2149.296	1395.926	1808.088	446.425	2079.405	-45.256
2500	1026.279	2191.106	1426.902	1910.510	447.908	2147.482	-44.868
2600	1030.047	2231.432	1457.075	2013.330	449.143	2215.385	-44.507
2700	1033.448	2270.371	1486.480	2116.507	450.137	2283.320	-44.173
2800	1036.527	2308.012	1515.152	2220.008	450.862	2351.244	-43.862
2900	1039.322	2344.435	1543.123	2323.803	451.289	2419.094	-43.572
3000	1041.867	2379.713	1570.425	2427.865	451.462	2486.960	-43.301
3100	1044.190	2413.914	1597.085	2532.169	451.303	2554.746	-43.046
3200	1046.316	2447.100	1623.132	2636.696	450.854	2622.618	-42.809
3300	1048.265	2479.327	1648.592	2741.426	450.096	2690.549	-42.587
3400	1050.056	2510.648	1673.488	2846.344	449.001	2758.419	-42.377
3500	1051.707	2541.110	1697.844	2951.433	447.575	2826.307	-42.179
3600	1053.230	2570.759	1721.681	3056.681	445.838	2894.330	-41.995
3700	1054.639	2599.636	1745.021	3162.075	443.761	2962.424	-41.821
3800	1055.944	2627.779	1767.883	3267.605	441.315	3030.516	-41.656
3900	1057.155	2655.224	1790.285	3373.261	438.542	3098.624	-41.501
4000	1058.282	2682.003	1812.245	3479.033	435.427	3166.951	-41.355
4100	1059.331	2708.148	1833.778	3584.915	431.932	3235.284	-41.217
4200	1060.309	2733.687	1854.902	3690.897	428.087	3303.697	-41.087
4300	1061.223	2758.647	1875.630	3796.974	423.876	3372.114	-40.962
4400	1062.078	2783.054	1895.977	3903.140	419.309	3440.727	-40.846
4500	1062.879	2806.931	1915.956	4009.388	414.402	3509.505	-40.736
4600	1063.631	2830.300	1935.580	4115.714	409.100	3578.406	-40.633
4700	1064.336	2853.183	1954.861	4222.113	403.418	3647.308	-40.534
4800	1065.000	2875.598	1973.810	4328.580	397.405	3716.444	-40.442
4900	1065.625	2897.564	1992.439	4435.111	390.985	3785.569	-40.354
5000	1066.214	2919.098	2010.757	4541.704	384.253	3855.022	-40.272

3.347. Dibenzo[*f,pqr*]picene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-42-9
Point Group: C₁

Length: 15.61 Å
Width: 11.06 Å
Breadth: 5.084 Å
L/B Ratio: 1.411

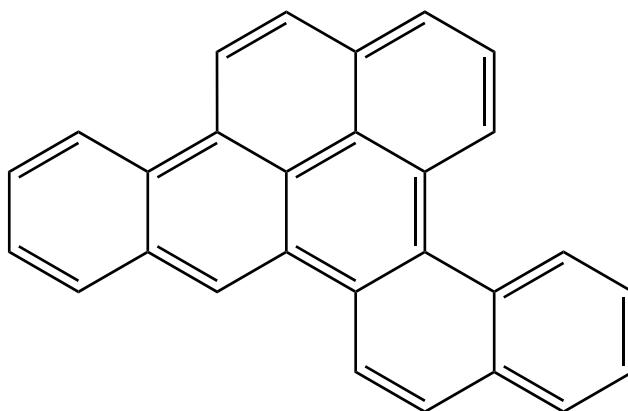
Cartesian coordinates:

C	-3.7437	-3.2744	-0.3740	C	1.3268	1.6816	-0.3044	H	-0.3861	-2.9964	-0.7814
C	-4.0392	-1.9620	-0.0672	C	2.3283	2.6937	-0.5402	H	-2.1852	-4.6601	-0.9413
C	-1.4160	-2.6907	-0.5517	C	3.6445	2.3965	-0.4926	H	-5.4794	0.0203	0.5407
C	-2.4220	-3.6321	-0.6478	C	4.0895	1.0592	-0.1854	H	-6.0920	2.4271	0.6948
C	-1.6803	-1.3602	-0.1743	C	5.4469	0.7463	-0.1090	H	-4.3499	4.1747	0.3745
C	-3.0275	-0.9872	-0.0002	C	5.8540	-0.5478	0.2057	H	-1.9936	3.5230	-0.0384
C	-2.3921	1.3933	0.0289	C	4.9194	-1.5415	0.4540	H	-0.3380	3.0457	-0.3963
C	-3.3832	0.4109	0.1718	C	1.7242	0.3466	-0.0457	H	1.9854	3.7110	-0.7616
C	-4.7121	0.8000	0.4202	C	3.1249	0.0499	0.0490	H	4.4063	3.1621	-0.6789
C	-5.0553	2.1344	0.4998	C	3.5506	-1.2534	0.3806	H	6.1954	1.5245	-0.2965
C	-4.0753	3.1161	0.3237	C	2.5512	-2.2465	0.6550	H	6.9228	-0.7799	0.2605
C	-2.7648	2.7492	0.0925	C	1.2333	-1.9633	0.5315	H	5.2455	-2.5558	0.7100
C	-0.6236	-0.3586	-0.0502	C	0.7546	-0.6669	0.1227	H	2.8843	-3.2399	0.9774
C	-0.9969	1.0005	-0.1195	H	-4.5379	-4.0261	-0.4219	H	0.4944	-2.7415	0.7674
C	-0.0223	1.9962	-0.2839	H	-5.0809	-1.6576	0.1171				

Table 3.347: Table of thermodynamic data as a function of temperature for Dibenzo[*f,pqr*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-51.634	464.321	464.321	∞
100	111.936	355.314	802.654	-44.734	491.079	538.795	-281.432
200	223.806	465.337	606.448	-28.222	476.911	592.162	-154.654
250	288.627	522.191	583.882	-15.423	470.254	621.744	-129.904
298.15	351.833	578.445	578.445	0.000	464.321	651.474	-114.133
300	354.233	580.628	578.451	0.653	464.102	652.634	-113.631
350	417.388	640.024	582.998	19.959	458.628	684.501	-102.154
400	476.023	699.644	593.854	42.316	453.873	717.092	-93.641
450	529.187	758.836	608.903	67.470	449.755	750.247	-87.085
500	576.735	817.101	626.819	95.141	446.186	783.851	-81.887
600	656.495	929.591	667.990	156.961	440.390	851.959	-74.168
700	719.566	1035.712	713.020	225.884	436.165	920.915	-68.718
800	770.131	1135.217	759.644	300.458	433.327	990.363	-64.663
900	811.319	1228.383	806.607	379.599	431.695	1060.087	-61.525
1000	845.332	1315.680	853.196	462.484	431.105	1129.949	-59.021
1100	873.725	1397.620	899.003	548.478	431.355	1199.837	-56.974
1200	897.635	1474.698	943.798	637.080	432.304	1269.653	-55.265
1300	917.917	1547.370	987.459	727.884	433.769	1339.378	-53.816
1400	935.230	1616.045	1029.928	820.564	435.617	1408.980	-52.569
1500	950.095	1681.089	1071.189	914.849	437.766	1478.441	-51.483
1600	962.928	1742.826	1111.254	1010.515	440.084	1547.742	-50.528
1700	974.062	1801.545	1150.146	1107.378	442.499	1616.871	-49.679
1800	983.770	1857.502	1187.902	1205.280	444.933	1685.922	-48.923
1900	992.273	1910.924	1224.560	1304.092	447.357	1754.784	-48.241
2000	999.754	1962.016	1260.165	1403.701	449.714	1823.547	-47.625
2100	1006.364	2010.957	1294.760	1504.014	451.927	1892.180	-47.064
2200	1012.227	2057.911	1328.389	1604.949	453.994	1960.714	-46.552
2300	1017.449	2103.024	1361.094	1706.438	455.911	2029.157	-46.083
2400	1022.115	2146.426	1392.918	1808.420	457.605	2097.471	-45.649
2500	1026.300	2188.238	1423.900	1910.845	459.090	2165.836	-45.252
2600	1030.065	2228.564	1454.077	2013.666	460.327	2234.025	-44.881
2700	1033.465	2267.504	1483.487	2116.846	461.322	2302.246	-44.539
2800	1036.542	2305.146	1512.164	2220.348	462.049	2370.458	-44.221
2900	1039.336	2341.569	1540.139	2324.145	462.477	2438.594	-43.923
3000	1041.879	2376.847	1567.445	2428.207	462.652	2506.746	-43.645
3100	1044.201	2411.049	1594.109	2532.513	462.494	2574.819	-43.385
3200	1046.325	2444.235	1620.160	2637.041	462.046	2642.978	-43.141
3300	1048.274	2476.462	1645.622	2741.772	461.289	2711.195	-42.914
3400	1050.065	2507.783	1670.521	2846.690	460.195	2779.351	-42.699
3500	1051.714	2538.246	1694.880	2951.781	458.769	2847.526	-42.496
3600	1053.237	2567.896	1718.721	3057.029	457.034	2915.836	-42.307
3700	1054.645	2596.773	1742.063	3162.424	454.957	2984.216	-42.129
3800	1055.950	2624.916	1764.928	3267.955	452.512	3052.594	-41.960
3900	1057.161	2652.360	1787.332	3373.611	449.740	3120.989	-41.800
4000	1058.287	2679.140	1809.294	3479.384	446.625	3189.602	-41.651
4100	1059.336	2705.285	1830.830	3585.266	443.131	3258.221	-41.509
4200	1060.314	2730.824	1851.955	3691.249	439.286	3326.921	-41.375
4300	1061.227	2755.784	1872.685	3797.326	435.075	3395.623	-41.248
4400	1062.082	2780.191	1893.034	3903.492	430.509	3464.523	-41.128
4500	1062.883	2804.068	1913.015	4009.741	425.602	3533.588	-41.016
4600	1063.634	2827.438	1932.641	4116.067	420.300	3602.774	-40.910
4700	1064.340	2850.320	1951.923	4222.466	414.619	3671.963	-40.808
4800	1065.003	2872.735	1970.874	4328.934	408.607	3741.385	-40.714
4900	1065.628	2894.701	1989.504	4435.466	402.187	3810.797	-40.623
5000	1066.217	2916.236	2007.824	4542.058	395.455	3880.536	-40.539

3.348. Benzo[*b*]naphtho[8,1,2-*pqr*]chrysene



Other names: Phenanthro[4,3,2,1-*def*]chrysene

Formula: C₂₈H₁₆

Mass: 352.427 g/mol

CAS Number: 137593-96-5

Point Group: C₁

Length: 16.01 Å

Width: 11.15 Å

Breadth: 4.969 Å

L/B Ratio: 1.436

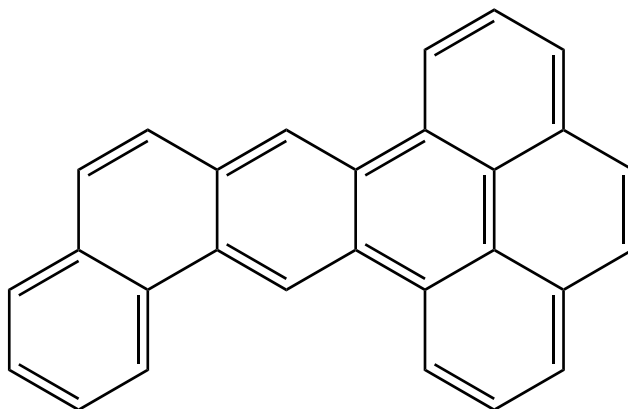
Cartesian coordinates:

C	5.2947	-2.3632	-0.1139	C	-5.3545	0.0137	-0.7586	H	5.1675	1.0393	-0.4435
C	5.7373	-1.0346	-0.2943	C	-5.7489	-1.3024	-0.4422	H	3.6092	-3.6585	0.1893
C	4.8375	-0.0017	-0.3053	C	-4.8109	-2.2029	-0.0147	H	1.3093	-2.8910	0.3383
C	3.9610	-2.6301	0.0495	C	-1.2293	1.2900	0.1911	H	-2.7994	-3.8229	0.6618
C	3.0110	-1.5745	0.0388	C	-0.3055	3.9637	0.2291	H	-0.3914	-3.2279	0.6394
C	3.4503	-0.2485	-0.1378	C	-1.6288	3.6764	0.4757	H	-3.7732	1.4394	-0.8527
C	1.6265	-1.8452	0.1990	C	-2.0833	2.3530	0.4581	H	-6.0991	0.7152	-1.1495
C	0.6914	-0.8375	0.1739	C	1.1254	0.5167	0.0130	H	-6.7974	-1.5950	-0.5571
C	-0.7399	-1.1139	0.2582	C	2.4854	0.8110	-0.1339	H	-5.0910	-3.2387	0.2089
C	-1.6842	-0.0999	0.1151	C	2.8992	2.1759	-0.2535	H	0.0492	5.0002	0.2050
C	-2.4773	-2.7957	0.4564	C	2.0002	3.1874	-0.1619	H	-2.3404	4.4837	0.6789
C	-1.1590	-2.4591	0.4630	C	0.6090	2.9109	0.0343	H	-3.1487	2.1717	0.6562
C	-3.4532	-1.8150	0.1301	C	0.1601	1.5738	0.0603	H	3.9714	2.3747	-0.4046
C	-3.0606	-0.4765	-0.0927	H	6.0295	-3.1748	-0.1068	H	2.3198	4.2335	-0.2307
C	-4.0547	0.4113	-0.5871	H	6.8069	-0.8404	-0.4247				

Table 3.348: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[8,1,2-*pqr*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.640	469.644	469.644	∞
100	112.295	353.938	801.660	-44.772	496.364	544.217	-284.264
200	223.969	464.208	605.340	-28.226	482.230	597.707	-156.102
250	288.656	521.082	582.772	-15.422	475.578	627.345	-131.074
298.15	351.800	577.335	577.335	0.000	469.644	657.128	-115.124
300	354.199	579.518	577.342	0.653	469.425	658.290	-114.616
350	417.325	638.906	581.888	19.957	463.949	690.213	-103.007
400	475.945	698.516	592.742	42.310	459.190	722.860	-94.394
450	529.101	757.699	607.789	67.460	455.068	756.071	-87.761
500	576.646	815.955	625.702	95.126	451.494	789.733	-82.501
600	656.404	928.428	666.866	156.937	445.689	857.956	-74.690
700	719.477	1034.535	711.890	225.851	441.455	927.029	-69.174
800	770.045	1134.029	758.507	300.417	438.609	996.596	-65.070
900	811.238	1227.185	805.464	379.549	436.969	1066.439	-61.893
1000	845.254	1314.473	852.047	462.426	436.370	1136.421	-59.359
1100	873.652	1396.406	897.849	548.413	436.613	1206.430	-57.287
1200	897.567	1473.478	942.639	637.007	437.555	1276.367	-55.558
1300	917.853	1546.145	986.294	727.806	439.014	1346.215	-54.090
1400	935.171	1614.815	1028.759	820.479	440.855	1415.939	-52.828
1500	950.040	1679.855	1070.016	914.758	442.998	1485.523	-51.729
1600	962.877	1741.589	1110.077	1010.419	445.312	1554.948	-50.763
1700	974.014	1800.305	1148.966	1107.277	447.721	1624.201	-49.905
1800	983.726	1856.259	1186.718	1205.175	450.151	1693.376	-49.139
1900	992.232	1909.680	1223.373	1303.982	452.570	1762.362	-48.450
2000	999.716	1960.769	1258.975	1403.587	454.923	1831.250	-47.826
2100	1006.328	2009.708	1293.567	1503.896	457.132	1900.008	-47.259
2200	1012.194	2056.661	1327.194	1604.828	459.196	1968.667	-46.741
2300	1017.417	2101.772	1359.897	1706.313	461.110	2037.235	-46.266
2400	1022.085	2145.173	1391.718	1808.293	462.801	2105.674	-45.828
2500	1026.272	2186.983	1422.698	1910.715	464.283	2174.164	-45.426
2600	1030.040	2227.309	1452.873	2013.533	465.518	2242.479	-45.051
2700	1033.440	2266.248	1482.281	2116.710	466.510	2310.826	-44.705
2800	1036.519	2303.888	1510.956	2220.211	467.235	2379.163	-44.383
2900	1039.314	2340.311	1538.930	2324.005	467.661	2447.425	-44.082
3000	1041.859	2375.589	1566.234	2428.065	467.833	2515.703	-43.801
3100	1044.182	2409.790	1592.896	2532.369	467.673	2583.902	-43.538
3200	1046.307	2442.975	1618.945	2636.895	467.223	2652.186	-43.292
3300	1048.256	2475.202	1644.407	2741.625	466.465	2720.530	-43.062
3400	1050.048	2506.522	1669.304	2846.541	465.369	2788.812	-42.844
3500	1051.699	2536.985	1693.662	2951.629	463.942	2857.113	-42.639
3600	1053.222	2566.634	1717.501	3056.877	462.205	2925.549	-42.448
3700	1054.631	2595.510	1740.843	3162.270	460.126	2994.055	-42.268
3800	1055.936	2623.653	1763.706	3267.799	457.679	3062.560	-42.097
3900	1057.148	2651.097	1786.109	3373.454	454.906	3131.081	-41.935
4000	1058.275	2677.876	1808.070	3479.226	451.790	3199.820	-41.785
4100	1059.324	2704.021	1829.605	3585.107	448.295	3268.565	-41.641
4200	1060.303	2729.560	1850.730	3691.088	444.449	3337.391	-41.506
4300	1061.217	2754.520	1871.459	3797.165	440.237	3406.221	-41.377
4400	1062.072	2778.927	1891.807	3903.330	435.670	3475.247	-41.256
4500	1062.873	2802.804	1911.787	4009.578	430.762	3544.438	-41.142
4600	1063.625	2826.173	1931.412	4115.903	425.459	3613.751	-41.035
4700	1064.331	2849.055	1950.693	4222.301	419.777	3683.066	-40.932
4800	1064.995	2871.470	1969.644	4328.768	413.764	3752.614	-40.836
4900	1065.620	2893.436	1988.273	4435.299	407.343	3822.153	-40.744
5000	1066.209	2914.970	2006.592	4541.890	400.610	3892.018	-40.659

3.349. Tribenzo[*a,hi,mn*]naphthacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 54961-30-7
Point Group: C_s

Length: 16.16 Å
Width: 11.13 Å
Breadth: 3.886 Å
L/B Ratio: 1.451

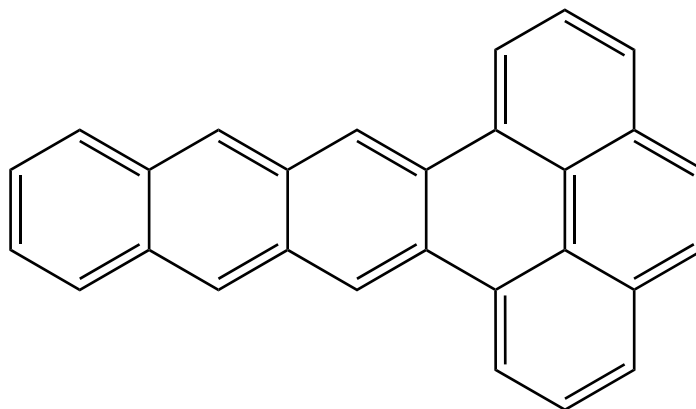
Cartesian coordinates:

C	6.3119	-1.0794	0.0000	C	-3.3227	-3.2080	0.0000	H	3.1598	-2.4002	0.0000
C	5.9966	0.2615	0.0000	C	-2.0090	-3.6375	0.0000	H	5.5554	-3.1076	0.0000
C	3.9716	-1.6566	0.0000	C	-0.9632	-2.7134	0.0000	H	5.1309	2.8026	0.0000
C	5.2928	-2.0447	0.0000	C	-1.8211	1.4682	0.0000	H	2.7611	3.5428	0.0000
C	3.6264	-0.2894	0.0000	C	-2.1456	2.8216	0.0000	H	0.3753	3.0143	0.0000
C	4.6485	0.6758	0.0000	C	-3.4777	3.2376	0.0000	H	1.4258	-1.8637	0.0000
C	4.3117	2.0743	0.0000	C	-4.5012	2.3088	0.0000	H	-4.1435	-3.9340	0.0000
C	3.0203	2.4778	0.0000	C	-2.5621	-0.8962	0.0000	H	-1.7817	-4.7087	0.0000
C	2.2438	0.1405	0.0000	C	-2.8622	0.5098	0.0000	H	0.0814	-3.0610	0.0000
C	1.9483	1.5186	0.0000	C	-4.2057	0.9354	0.0000	H	-1.3346	3.5661	0.0000
C	0.6101	1.9373	0.0000	C	-5.2583	-0.0453	0.0000	H	-3.7079	4.3082	0.0000
C	1.1885	-0.7822	0.0000	C	-4.9758	-1.3686	0.0000	H	-5.5470	2.6361	0.0000
C	-0.1380	-0.3682	0.0000	C	-3.6144	-1.8338	0.0000	H	-6.2950	0.3108	0.0000
C	-0.4333	1.0186	0.0000	H	7.3587	-1.4004	0.0000	H	-5.7766	-2.1170	0.0000
C	-1.2205	-1.3457	0.0000	H	6.7892	1.0185	0.0000				

Table 3.349: Table of thermodynamic data as a function of temperature for Tribenzo[*a,hi,mn*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.646	431.176	431.176	∞
100	112.371	358.558	805.242	-44.668	458.000	505.391	-263.984
200	223.411	468.585	609.389	-28.161	443.827	558.429	-145.844
250	287.991	525.324	586.873	-15.387	437.145	587.852	-122.822
298.15	351.001	581.449	581.449	0.000	431.176	617.434	-108.170
300	353.394	583.627	581.455	0.652	430.956	618.588	-107.703
350	416.388	642.881	585.991	19.911	425.435	650.309	-97.051
400	474.913	702.359	596.821	42.215	420.627	682.760	-89.158
450	528.019	761.417	611.835	67.312	416.452	715.783	-83.084
500	575.553	819.557	629.709	94.924	412.824	749.261	-78.273
600	655.375	931.836	670.789	156.628	406.912	817.134	-71.136
700	718.568	1037.793	715.728	225.445	402.581	885.874	-66.103
800	769.269	1137.174	762.266	299.927	399.651	955.121	-62.362
900	810.586	1230.246	809.149	378.987	397.939	1024.654	-59.468
1000	844.711	1317.471	855.667	461.805	397.281	1094.333	-57.161
1100	873.199	1399.357	901.410	547.742	397.474	1164.046	-55.275
1200	897.188	1476.393	946.147	636.295	398.375	1233.689	-53.700
1300	917.534	1549.031	989.756	727.058	399.798	1303.247	-52.364
1400	934.901	1617.680	1032.178	819.702	401.610	1372.684	-51.214
1500	949.810	1682.703	1073.398	913.957	403.729	1441.982	-50.213
1600	962.679	1744.423	1113.425	1009.597	406.021	1511.123	-49.332
1700	973.844	1803.128	1152.283	1106.436	408.412	1580.093	-48.549
1800	983.577	1859.073	1190.008	1204.318	410.826	1648.986	-47.851
1900	992.102	1912.486	1226.638	1303.111	413.231	1717.692	-47.222
2000	999.601	1963.569	1262.217	1402.704	415.572	1786.299	-46.652
2100	1006.227	2012.503	1296.788	1503.002	417.770	1854.777	-46.134
2200	1012.103	2059.451	1330.394	1603.924	419.824	1923.157	-45.661
2300	1017.336	2104.558	1363.080	1705.401	421.729	1991.446	-45.226
2400	1022.012	2147.956	1394.884	1807.373	423.413	2059.607	-44.825
2500	1026.206	2189.764	1425.849	1909.788	424.888	2127.819	-44.457
2600	1029.979	2230.087	1456.010	2012.600	426.116	2195.856	-44.114
2700	1033.385	2269.024	1485.405	2115.771	427.103	2263.925	-43.797
2800	1036.469	2306.662	1514.067	2219.266	427.822	2331.985	-43.503
2900	1039.268	2343.083	1542.029	2323.055	428.243	2399.969	-43.227
3000	1041.816	2378.359	1569.322	2427.112	428.412	2467.970	-42.970
3100	1044.142	2412.559	1595.974	2531.411	428.247	2535.892	-42.729
3200	1046.271	2445.743	1622.014	2635.934	427.794	2603.900	-42.503
3300	1048.222	2477.969	1647.466	2740.660	427.032	2671.967	-42.293
3400	1050.016	2509.288	1672.355	2845.573	425.933	2739.972	-42.094
3500	1051.669	2539.750	1696.705	2950.658	424.502	2807.996	-41.906
3600	1053.194	2569.398	1720.536	3055.902	422.762	2876.156	-41.731
3700	1054.605	2598.274	1743.870	3161.293	420.681	2944.385	-41.566
3800	1055.912	2626.416	1766.726	3266.820	418.232	3012.614	-41.410
3900	1057.125	2653.859	1789.123	3372.472	415.456	3080.859	-41.263
4000	1058.253	2680.638	1811.077	3478.242	412.338	3149.322	-41.125
4100	1059.303	2706.782	1832.606	3584.120	408.840	3217.791	-40.994
4200	1060.283	2732.321	1853.725	3690.100	404.992	3286.341	-40.871
4300	1061.198	2757.280	1874.449	3796.175	400.779	3354.894	-40.753
4400	1062.054	2781.687	1894.792	3902.338	396.210	3423.644	-40.643
4500	1062.856	2805.563	1914.767	4008.584	391.300	3492.559	-40.540
4600	1063.609	2828.932	1934.387	4114.908	385.996	3561.597	-40.442
4700	1064.315	2851.814	1953.664	4221.304	380.312	3630.636	-40.349
4800	1064.980	2874.228	1972.610	4327.769	374.297	3699.909	-40.262
4900	1065.606	2896.194	1991.235	4434.299	367.875	3769.171	-40.179
5000	1066.195	2917.728	2009.550	4540.889	361.141	3838.761	-40.102

3.350. Dibenzo[*de,uv*]pentacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 193-11-3
Point Group: C_{2v}

Length: 16.72 Å
Width: 11.36 Å
Breadth: 3.890 Å
L/B Ratio: 1.472

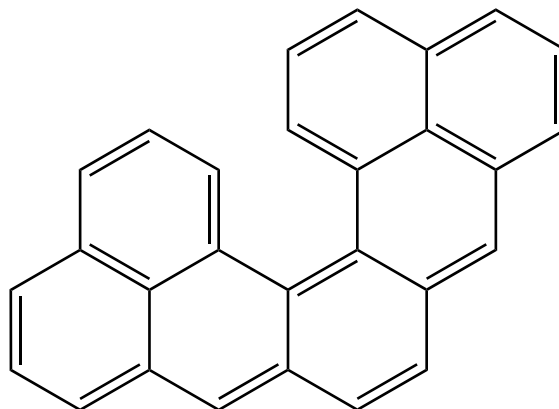
Cartesian coordinates:

C	-6.8783	0.7094	0.0000	C	1.7244	-2.8304	0.0000	H	-5.6966	-2.5035	0.0000
C	-6.8775	-0.7170	0.0000	C	2.9428	-3.5150	0.0000	H	-5.6993	2.4972	0.0000
C	-5.7071	-1.4076	0.0000	C	4.1343	-2.8189	0.0000	H	-3.2396	-2.5037	0.0000
C	-5.7086	1.4013	0.0000	C	1.6846	1.4427	0.0000	H	-3.2423	2.5001	0.0000
C	-4.4521	0.7093	0.0000	C	4.1311	2.8236	0.0000	H	-0.7781	-2.4997	0.0000
C	-4.4513	-0.7143	0.0000	C	2.9388	3.5184	0.0000	H	-0.7809	2.4988	0.0000
C	-3.2413	-1.4068	0.0000	C	1.7212	2.8323	0.0000	H	0.7783	-3.3933	0.0000
C	-3.2428	1.4032	0.0000	C	2.9026	0.7210	0.0000	H	2.9447	-4.6101	0.0000
C	-2.0266	0.7091	0.0000	C	2.9034	-0.7178	0.0000	H	5.0907	-3.3539	0.0000
C	-2.0259	-0.7113	0.0000	C	4.1285	-1.4121	0.0000	H	5.0870	3.3596	0.0000
C	-0.7773	-1.3974	0.0000	C	5.3622	-0.6737	0.0000	H	2.9394	4.6134	0.0000
C	-0.7789	1.3965	0.0000	C	5.3615	0.6796	0.0000	H	0.7744	3.3941	0.0000
C	0.4149	0.7192	0.0000	C	4.1269	1.4167	0.0000	H	6.3018	-1.2381	0.0000
C	0.4157	-0.7187	0.0000	H	-7.8399	1.2331	0.0000	H	6.3005	1.2451	0.0000
C	1.6863	-1.4409	0.0000	H	-7.8385	-1.2417	0.0000				

Table 3.350: Table of thermodynamic data as a function of temperature for Dibenzo[de,uv]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-51.639	456.099	456.099	∞
100	111.836	350.582	797.971	-44.739	482.852	531.041	-277.381
200	223.846	460.550	601.722	-28.234	468.676	584.885	-152.753
250	288.768	517.426	579.145	-15.430	462.025	614.706	-128.433
298.15	351.970	573.705	573.705	0.000	456.099	644.665	-112.940
300	354.369	575.890	573.712	0.653	455.880	645.833	-112.447
350	417.441	635.301	578.260	19.964	450.411	677.937	-101.175
400	475.969	694.921	589.118	42.321	445.656	710.764	-92.814
450	529.035	754.101	604.168	67.470	441.532	744.155	-86.378
500	576.513	812.346	622.083	95.131	437.954	777.997	-81.275
600	656.213	924.788	663.246	156.925	432.132	846.583	-73.700
700	719.300	1030.866	708.265	225.821	427.879	916.021	-68.353
800	769.917	1130.339	754.876	300.371	425.017	985.956	-64.375
900	811.166	1223.483	801.825	379.493	423.367	1056.169	-61.297
1000	845.234	1310.767	848.402	462.365	422.764	1126.521	-58.842
1100	873.675	1392.700	894.198	548.352	423.007	1196.901	-56.835
1200	897.621	1469.775	938.983	636.951	423.953	1267.208	-55.159
1300	917.930	1542.447	982.635	727.756	425.418	1337.426	-53.737
1400	935.264	1611.124	1025.097	820.438	427.268	1407.520	-52.514
1500	950.144	1676.171	1066.353	914.727	429.421	1477.473	-51.449
1600	962.986	1737.912	1106.413	1010.399	431.745	1547.266	-50.512
1700	974.127	1796.635	1145.301	1107.267	434.166	1616.886	-49.680
1800	983.838	1852.595	1183.053	1205.176	436.607	1686.428	-48.938
1900	992.343	1906.021	1219.708	1303.995	439.037	1755.780	-48.269
2000	999.825	1957.116	1255.311	1403.611	441.402	1825.033	-47.664
2100	1006.434	2006.061	1289.904	1503.931	443.621	1894.156	-47.114
2200	1012.296	2053.018	1323.531	1604.873	445.695	1963.180	-46.611
2300	1017.516	2098.134	1356.235	1706.368	447.619	2032.112	-46.150
2400	1022.180	2141.540	1388.057	1808.357	449.320	2100.915	-45.724
2500	1026.363	2183.353	1419.038	1910.788	450.811	2169.768	-45.334
2600	1030.126	2223.683	1449.215	2013.616	452.055	2238.446	-44.970
2700	1033.523	2262.625	1478.624	2116.801	453.056	2307.155	-44.634
2800	1036.598	2300.268	1507.300	2220.310	453.789	2375.854	-44.321
2900	1039.390	2336.693	1535.275	2324.112	454.222	2444.478	-44.029
3000	1041.931	2371.973	1562.580	2428.180	454.402	2513.118	-43.756
3100	1044.251	2406.177	1589.244	2532.490	454.249	2581.678	-43.500
3200	1046.373	2439.364	1615.294	2637.023	453.806	2650.324	-43.261
3300	1048.320	2471.593	1640.757	2741.759	453.054	2719.028	-43.038
3400	1050.108	2502.915	1665.656	2846.682	451.964	2787.671	-42.826
3500	1051.756	2533.380	1690.015	2951.776	450.543	2856.332	-42.628
3600	1053.277	2563.030	1713.855	3057.029	448.811	2925.129	-42.442
3700	1054.684	2591.908	1737.198	3162.428	446.738	2993.995	-42.267
3800	1055.987	2620.052	1760.062	3267.962	444.297	3062.861	-42.101
3900	1057.197	2647.498	1782.467	3373.622	441.529	3131.741	-41.944
4000	1058.321	2674.278	1804.428	3479.399	438.417	3200.841	-41.798
4100	1059.369	2700.424	1825.964	3585.284	434.926	3269.946	-41.659
4200	1060.345	2725.964	1847.090	3691.270	431.085	3339.131	-41.527
4300	1061.258	2750.925	1867.820	3797.351	426.877	3408.320	-41.402
4400	1062.112	2775.333	1888.169	3903.520	422.314	3477.706	-41.285
4500	1062.911	2799.211	1908.150	4009.771	417.410	3547.256	-41.175
4600	1063.662	2822.581	1927.776	4116.100	412.111	3616.928	-41.071
4700	1064.366	2845.464	1947.059	4222.502	406.433	3686.603	-40.971
4800	1065.029	2867.879	1966.010	4328.972	400.423	3756.510	-40.878
4900	1065.652	2889.846	1984.640	4435.506	394.005	3826.408	-40.789
5000	1066.240	2911.381	2002.960	4542.101	387.276	3896.632	-40.707

3.351. Dibenzo[*pq,uv*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 137593-97-6
Point Group: C₂

Length: 15.85 Å
Width: 10.37 Å
Breadth: 5.320 Å
L/B Ratio: 1.528

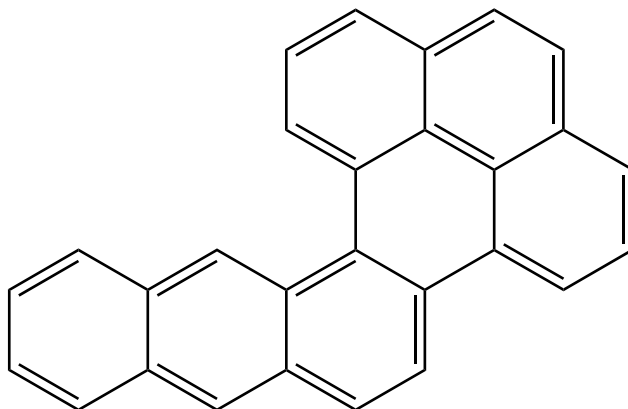
Cartesian coordinates:

C	2.8081	2.7144	0.0292	C	-4.9556	-0.9670	-0.0400	H	-5.4952	-1.9203	-0.0684
C	3.5599	1.4689	-0.0192	C	-5.6317	0.2210	-0.0376	H	-3.3638	-3.1499	-0.0416
C	2.8305	0.2389	-0.0563	C	-4.9331	1.4516	-0.0210	H	-1.2374	-4.3721	-0.0421
C	1.4178	0.2366	-0.1251	C	-2.8129	-2.2017	-0.0231	H	1.2375	-4.3721	0.0423
C	0.6686	1.5119	-0.3819	C	-1.4300	-2.1971	-0.0211	H	3.3638	-3.1499	0.0415
C	1.4768	2.7334	-0.0970	C	1.4300	-2.1970	0.0212	H	5.4951	-1.9203	0.0679
C	0.7256	-0.9620	-0.0200	C	0.6733	-3.4324	0.0209	H	6.7265	0.2374	0.0581
C	-0.7256	-0.9620	0.0202	C	-0.6733	-3.4324	-0.0207	H	5.4998	2.3890	0.0505
C	-1.4178	0.2365	0.1253	C	3.5315	-0.9867	0.0049	H	3.3770	3.6373	0.1916
C	-0.6686	1.5118	0.3821	C	2.8129	-2.2016	0.0231	H	0.9028	3.6708	-0.0283
C	-1.4769	2.7334	0.0972	C	4.9330	1.4517	0.0208	H	0.4488	1.5345	-1.4821
C	-2.8082	2.7143	-0.0291	C	5.6318	0.2210	0.0373	H	-0.4488	1.5345	1.4822
C	-3.5600	1.4688	0.0192	C	4.9557	-0.9669	0.0397	H	-0.9028	3.6708	0.0286
C	-2.8305	0.2389	0.0563	H	-5.4997	2.3890	-0.0508	H	-3.3770	3.6372	-0.1915
C	-3.5315	-0.9867	-0.0050	H	-6.7265	0.2373	-0.0587				

Table 3.351: Table of thermodynamic data as a function of temperature for Dibenzop[*pq,uv*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-49.796	579.070	579.070	∞
100	103.007	335.513	770.985	-43.547	607.015	656.711	-343.023
200	218.139	440.421	579.191	-27.754	592.128	712.362	-186.046
250	283.911	496.119	556.969	-15.212	585.214	743.222	-155.284
298.15	347.788	551.602	551.602	0.000	579.070	774.226	-135.638
300	350.211	553.761	551.609	0.646	578.844	775.436	-135.013
350	413.931	612.580	556.109	19.765	573.183	808.662	-120.684
400	473.057	671.771	566.867	41.962	568.268	842.636	-110.035
450	526.665	730.640	581.799	66.978	564.012	877.193	-101.820
500	574.628	788.661	599.593	94.534	560.328	912.213	-95.296
600	655.149	900.835	640.532	156.182	554.360	983.183	-85.592
700	718.884	1006.800	685.365	225.005	550.035	1055.023	-78.725
800	769.993	1106.251	731.827	299.539	547.157	1127.366	-73.608
900	811.600	1199.426	778.662	378.687	545.533	1199.986	-69.644
1000	845.916	1286.769	825.152	461.617	544.987	1272.742	-66.480
1100	874.516	1368.775	870.884	547.681	545.307	1345.518	-63.892
1200	898.558	1445.928	915.621	636.368	546.342	1418.214	-61.732
1300	918.914	1518.677	959.239	727.270	547.904	1490.813	-59.900
1400	936.262	1587.428	1001.677	820.051	549.853	1563.280	-58.325
1500	951.133	1652.543	1042.917	914.439	552.105	1635.599	-56.955
1600	963.952	1714.347	1082.966	1010.209	554.527	1707.751	-55.751
1700	975.061	1773.128	1121.849	1107.173	557.043	1779.724	-54.683
1800	984.734	1829.141	1159.600	1205.174	559.576	1851.614	-53.731
1900	993.199	1882.614	1196.257	1304.080	562.094	1923.310	-52.874
2000	1000.639	1933.752	1231.862	1403.779	564.541	1994.901	-52.100
2100	1007.207	1982.735	1266.460	1504.178	566.840	2066.359	-51.397
2200	1013.028	2029.728	1300.093	1605.196	568.990	2137.714	-50.755
2300	1018.209	2074.875	1332.804	1706.763	570.985	2208.973	-50.166
2400	1022.836	2118.309	1364.635	1808.819	572.753	2280.100	-49.624
2500	1026.984	2160.149	1395.624	1911.314	574.308	2351.275	-49.126
2600	1030.715	2200.502	1425.809	2014.202	575.612	2422.272	-48.663
2700	1034.080	2239.466	1455.227	2117.445	576.671	2493.298	-48.235
2800	1037.126	2277.129	1483.912	2221.007	577.457	2564.313	-47.837
2900	1039.891	2313.572	1511.896	2324.860	577.942	2635.249	-47.465
3000	1042.406	2348.869	1539.210	2428.977	578.171	2706.200	-47.118
3100	1044.702	2383.087	1565.883	2533.334	578.064	2777.070	-46.792
3200	1046.802	2416.289	1591.942	2637.911	577.665	2848.024	-46.488
3300	1048.727	2448.531	1617.413	2742.689	576.955	2919.036	-46.204
3400	1050.497	2479.865	1642.320	2847.651	575.905	2989.984	-45.935
3500	1052.126	2510.340	1666.687	2952.784	574.522	3060.950	-45.681
3600	1053.630	2540.001	1690.536	3058.073	572.827	3132.050	-45.444
3700	1055.021	2568.888	1713.887	3163.506	570.788	3203.219	-45.220
3800	1056.309	2597.041	1736.759	3269.073	568.379	3274.385	-45.009
3900	1057.504	2624.495	1759.171	3374.765	565.643	3345.567	-44.808
4000	1058.615	2651.283	1781.140	3480.571	562.561	3416.966	-44.620
4100	1059.650	2677.436	1802.683	3586.485	559.099	3488.370	-44.441
4200	1060.615	2702.982	1823.816	3692.499	555.285	3559.855	-44.272
4300	1061.517	2727.950	1844.553	3798.606	551.104	3631.341	-44.111
4400	1062.360	2752.363	1864.909	3904.800	546.566	3703.024	-43.960
4500	1063.150	2776.247	1884.896	4011.076	541.686	3774.871	-43.817
4600	1063.891	2799.622	1904.528	4117.429	536.411	3846.839	-43.681
4700	1064.587	2822.509	1923.817	4223.853	530.755	3918.809	-43.552
4800	1065.241	2844.930	1942.774	4330.345	524.767	3991.012	-43.430
4900	1065.857	2866.900	1961.411	4436.900	518.370	4063.204	-43.313
5000	1066.437	2888.439	1979.737	4543.515	511.661	4135.723	-43.205

3.352. Dibenzo[*de,uv*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-48-5
Point Group: C₁

Length: 15.94 Å
Width: 10.41 Å
Breadth: 5.103 Å
L/B Ratio: 1.531

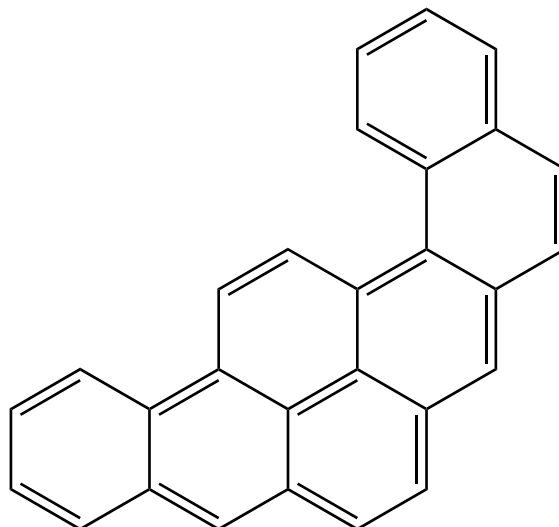
Cartesian coordinates:

C	5.8454	1.3684	-0.6687	C	-2.1103	3.4620	0.3868	H	6.0667	-1.9191	0.2571
C	6.4233	0.1105	-0.3358	C	-0.7701	3.3882	0.7248	H	4.0425	2.5028	-0.9026
C	5.6335	-0.9455	0.0020	C	-0.0957	2.1716	0.6869	H	3.8007	-2.8641	0.5341
C	4.4948	1.5380	-0.6466	C	-2.2580	-1.4089	0.0008	H	1.8303	1.5980	-0.4952
C	3.6341	0.4525	-0.2854	C	-3.0295	-2.5674	-0.1230	H	1.6045	-3.8277	0.7334
C	4.2101	-0.8029	0.0292	C	-4.3937	-2.4934	-0.3834	H	-0.8525	-3.6212	0.4598
C	3.3667	-1.8772	0.3299	C	-5.0197	-1.2635	-0.5138	H	-2.6318	4.4257	0.3855
C	2.2438	0.6127	-0.2348	C	-2.1332	1.0487	0.0698	H	-0.2312	4.2938	1.0232
C	1.3932	-0.4320	0.1286	C	-2.8918	-0.1529	-0.1195	H	0.9670	2.1583	0.9657
C	1.9830	-1.7119	0.3500	C	-4.2798	-0.0837	-0.3731	H	-2.5478	-3.5509	-0.0167
C	1.1388	-2.8568	0.5292	C	-4.9166	1.2044	-0.4591	H	-4.9755	-3.4156	-0.4851
C	-0.2016	-2.7359	0.3976	C	-4.2139	2.3375	-0.2378	H	-6.0948	-1.2093	-0.7190
C	-0.0531	-0.2983	0.2120	C	-2.8075	2.2905	0.0696	H	-5.9863	1.2371	-0.6955
C	-0.8196	-1.4560	0.2045	H	6.5090	2.1953	-0.9423	H	-4.6970	3.3204	-0.2842
C	-0.7352	0.9892	0.3048	H	7.5134	0.0103	-0.3586				

Table 3.352: Table of thermodynamic data as a function of temperature for Dibenzo[de,uv]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-51.471	472.251	472.251	∞
100	110.744	352.931	799.666	-44.674	499.070	547.024	-285.730
200	223.574	462.422	603.586	-28.233	484.830	600.664	-156.874
250	288.765	519.266	581.007	-15.435	478.172	630.394	-131.711
298.15	352.191	575.565	575.565	0.000	472.251	660.263	-115.673
300	354.598	577.751	575.572	0.654	472.033	661.428	-115.163
350	417.859	637.212	580.123	19.981	466.580	693.438	-103.488
400	476.524	696.897	590.991	42.362	461.850	726.168	-94.826
450	529.677	756.148	606.057	67.541	457.756	759.458	-88.154
500	577.198	814.463	623.991	95.236	454.211	793.196	-82.863
600	656.894	927.032	665.200	157.099	448.458	861.563	-75.004
700	719.913	1033.210	710.268	226.059	444.271	930.772	-69.454
800	770.440	1132.759	756.926	300.667	441.466	1000.468	-65.323
900	811.601	1225.960	803.920	379.836	439.864	1070.436	-62.125
1000	845.592	1313.285	850.537	462.748	439.300	1140.539	-59.574
1100	873.967	1395.249	896.369	548.768	439.575	1210.665	-57.489
1200	897.860	1472.348	941.187	637.393	440.548	1280.717	-55.747
1300	918.126	1545.037	984.868	728.219	442.035	1350.676	-54.270
1400	935.425	1613.727	1027.356	820.919	443.902	1420.510	-52.999
1500	950.276	1678.784	1068.635	915.223	446.070	1490.202	-51.892
1600	963.096	1740.532	1108.716	1010.907	448.406	1559.733	-50.919
1700	974.219	1799.261	1147.623	1107.785	450.837	1629.091	-50.055
1800	983.916	1855.227	1185.392	1205.703	453.286	1698.370	-49.284
1900	992.409	1908.657	1222.063	1304.529	455.724	1767.459	-48.590
2000	999.881	1959.755	1257.679	1404.151	458.094	1836.448	-47.962
2100	1006.483	2008.702	1292.285	1504.476	460.319	1905.308	-47.391
2200	1012.338	2055.662	1325.924	1605.423	462.398	1974.067	-46.869
2300	1017.552	2100.779	1358.639	1706.922	464.325	2042.735	-46.391
2400	1022.212	2144.186	1390.472	1808.915	466.030	2111.273	-45.950
2500	1026.391	2186.001	1421.462	1911.349	467.524	2179.861	-45.545
2600	1030.151	2226.331	1451.647	2014.179	468.770	2248.274	-45.167
2700	1033.545	2265.274	1481.064	2117.367	469.774	2316.719	-44.819
2800	1036.618	2302.918	1509.748	2220.877	470.508	2385.153	-44.495
2900	1039.407	2339.344	1537.730	2324.681	470.944	2453.511	-44.192
3000	1041.947	2374.625	1565.042	2428.750	471.126	2521.886	-43.909
3100	1044.265	2408.829	1591.712	2533.063	470.974	2590.181	-43.643
3200	1046.386	2442.017	1617.768	2637.597	470.532	2658.562	-43.396
3300	1048.331	2474.246	1643.236	2742.334	469.781	2727.001	-43.164
3400	1050.119	2505.569	1668.140	2847.258	468.693	2795.379	-42.945
3500	1051.766	2536.033	1692.504	2952.353	467.272	2863.775	-42.739
3600	1053.286	2565.684	1716.349	3057.607	465.542	2932.306	-42.546
3700	1054.692	2594.562	1739.696	3163.007	463.470	3000.907	-42.364
3800	1055.994	2622.707	1762.564	3268.542	461.029	3069.506	-42.192
3900	1057.204	2650.152	1784.972	3374.202	458.262	3138.122	-42.030
4000	1058.328	2676.933	1806.938	3479.980	455.151	3206.956	-41.878
4100	1059.374	2703.079	1828.477	3585.865	451.661	3275.795	-41.733
4200	1060.351	2728.619	1849.606	3691.852	447.819	3344.715	-41.597
4300	1061.263	2753.580	1870.340	3797.933	443.613	3413.639	-41.467
4400	1062.116	2777.988	1890.692	3904.103	439.050	3482.759	-41.345
4500	1062.916	2801.866	1910.676	4010.355	434.146	3552.044	-41.230
4600	1063.666	2825.236	1930.305	4116.684	428.848	3621.450	-41.122
4700	1064.370	2848.119	1949.590	4223.086	423.170	3690.859	-41.018
4800	1065.032	2870.535	1968.544	4329.557	417.160	3760.501	-40.922
4900	1065.656	2892.501	1987.176	4436.092	410.743	3830.133	-40.829
5000	1066.244	2914.036	2005.499	4542.687	404.014	3900.092	-40.743

3.353. Dibenzo[*a,rst*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-51-0
Point Group: C₁

Length: 16.24 Å
Width: 10.56 Å
Breadth: 4.794 Å
L/B Ratio: 1.538

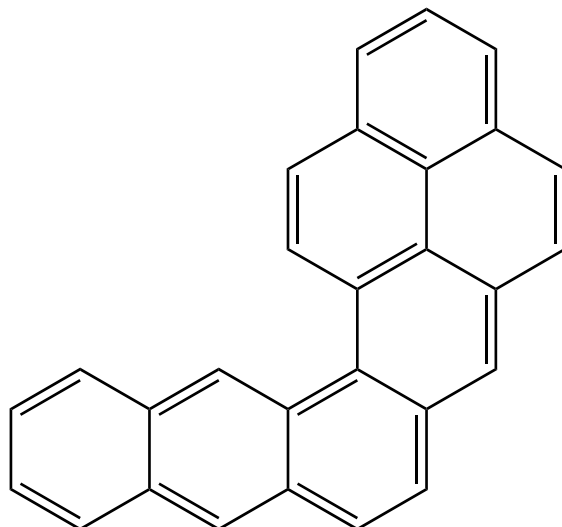
Cartesian coordinates:

C	-5.2074	-2.5809	-0.2187	C	-1.0145	-1.6715	-0.3701	H	-6.4311	0.5625	0.3010
C	-6.1403	-1.5425	-0.0117	C	-1.9956	-0.6639	-0.1445	H	-3.1236	-3.1016	-0.4290
C	-5.7124	-0.2492	0.1410	C	-1.5688	0.6576	0.0202	H	-4.6213	2.1934	0.3875
C	-3.8655	-2.3048	-0.2660	C	2.1908	0.2805	-0.0643	H	-2.8328	3.8485	0.4755
C	-3.3951	-0.9770	-0.1069	C	2.5405	1.6395	-0.1590	H	-0.4188	4.4044	0.3438
C	-4.3280	0.0591	0.0944	C	3.9022	2.0368	-0.3757	H	1.8792	3.7066	-0.0769
C	-3.8773	1.4002	0.2424	C	4.8893	1.1140	-0.4376	H	1.0359	-2.1762	-0.5688
C	-2.5385	1.7002	0.2010	C	3.2732	-0.6771	0.0799	H	-1.3678	-2.6977	-0.5568
C	-2.0775	3.0677	0.3288	C	4.5995	-0.2629	-0.1667	H	4.1177	3.1030	-0.5133
C	-0.7680	3.3686	0.2603	C	5.6669	-1.1852	-0.0868	H	5.9246	1.4016	-0.6537
C	0.2317	2.3365	0.0781	C	5.4393	-2.4842	0.2990	H	6.6820	-0.8462	-0.3242
C	1.5615	2.6563	-0.0587	C	4.1381	-2.8847	0.6408	H	6.2634	-3.2020	0.3606
C	-0.1712	0.9692	0.0018	C	3.0875	-2.0029	0.5371	H	3.9655	-3.9059	0.9967
C	0.7942	-0.0512	-0.1179	H	-5.5675	-3.6074	-0.3419	H	2.0852	-2.3400	0.8342
C	0.3131	-1.3753	-0.3618	H	-7.2079	-1.7827	0.0247				

Table 3.353: Table of thermodynamic data as a function of temperature for Dibenz[*a,rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.582	464.967	464.967	∞
100	111.306	353.993	801.472	-44.748	491.711	539.559	-281.831
200	223.948	463.815	605.118	-28.261	477.518	593.073	-154.892
250	289.045	520.733	582.519	-15.447	470.876	622.731	-130.110
298.15	352.387	577.073	577.073	0.000	464.967	652.529	-114.318
300	354.790	579.261	577.080	0.654	464.749	653.691	-113.815
350	417.981	638.746	581.634	19.989	459.304	685.625	-102.322
400	476.592	698.443	592.505	42.375	454.578	718.277	-93.795
450	529.707	757.700	607.575	67.556	450.487	751.490	-87.229
500	577.202	816.017	625.513	95.252	446.943	785.150	-82.022
600	656.872	928.584	666.727	157.114	441.189	853.363	-74.290
700	719.886	1034.758	711.798	226.072	436.999	922.416	-68.830
800	770.417	1134.303	758.458	300.676	434.191	991.958	-64.767
900	811.585	1227.502	805.453	379.844	432.587	1061.772	-61.622
1000	845.582	1314.826	852.071	462.755	432.022	1131.720	-59.114
1100	873.964	1396.789	897.904	548.774	432.297	1201.693	-57.062
1200	897.862	1473.887	942.722	637.398	433.269	1271.590	-55.350
1300	918.132	1546.577	986.404	728.225	434.756	1341.396	-53.897
1400	935.433	1615.268	1028.892	820.926	436.625	1411.076	-52.647
1500	950.287	1680.325	1070.171	915.231	438.793	1480.614	-51.558
1600	963.108	1742.074	1110.252	1010.916	441.130	1549.991	-50.601
1700	974.232	1800.804	1149.160	1107.796	443.562	1619.194	-49.751
1800	983.929	1856.770	1186.929	1205.715	446.013	1688.319	-48.993
1900	992.422	1910.201	1223.601	1304.541	448.452	1757.253	-48.309
2000	999.894	1961.300	1259.217	1404.165	450.824	1826.088	-47.692
2100	1006.495	2010.248	1293.823	1504.491	453.050	1894.793	-47.129
2200	1012.350	2057.208	1327.463	1605.439	455.130	1963.398	-46.616
2300	1017.564	2102.326	1360.178	1706.940	457.059	2031.910	-46.145
2400	1022.224	2145.733	1392.011	1808.934	458.764	2100.294	-45.711
2500	1026.402	2187.549	1423.001	1911.369	460.259	2168.728	-45.312
2600	1030.162	2227.879	1453.187	2014.200	461.507	2236.986	-44.941
2700	1033.555	2266.823	1482.605	2117.389	462.512	2305.276	-44.597
2800	1036.628	2304.467	1511.288	2220.900	463.247	2373.555	-44.278
2900	1039.417	2340.893	1539.271	2324.705	463.684	2441.758	-43.980
3000	1041.956	2376.175	1566.583	2428.775	463.866	2509.979	-43.702
3100	1044.274	2410.378	1593.253	2533.089	463.715	2578.119	-43.440
3200	1046.394	2443.567	1619.309	2637.624	463.274	2646.344	-43.196
3300	1048.339	2475.796	1644.778	2742.362	462.524	2714.628	-42.968
3400	1050.127	2507.119	1669.682	2847.286	461.437	2782.851	-42.752
3500	1051.773	2537.584	1694.046	2952.382	460.017	2851.092	-42.549
3600	1053.293	2567.235	1717.891	3057.637	458.287	2919.468	-42.359
3700	1054.699	2596.113	1741.238	3163.037	456.216	2987.914	-42.181
3800	1056.001	2624.258	1764.107	3268.573	453.776	3056.358	-42.012
3900	1057.210	2651.704	1786.516	3374.234	451.009	3124.818	-41.851
4000	1058.334	2678.484	1808.481	3480.012	447.899	3193.497	-41.702
4100	1059.380	2704.630	1830.021	3585.898	444.409	3262.181	-41.560
4200	1060.356	2730.171	1851.150	3691.886	440.568	3330.946	-41.426
4300	1061.268	2755.132	1871.884	3797.967	436.362	3399.715	-41.297
4400	1062.122	2779.540	1892.236	3904.137	431.800	3468.679	-41.178
4500	1062.921	2803.418	1912.220	4010.390	426.897	3537.809	-41.065
4600	1063.670	2826.788	1931.849	4116.720	421.599	3607.061	-40.959
4700	1064.375	2849.671	1951.135	4223.123	415.921	3676.314	-40.857
4800	1065.037	2872.087	1970.089	4329.593	409.912	3745.801	-40.762
4900	1065.660	2894.054	1988.722	4436.129	403.495	3815.278	-40.671
5000	1066.248	2915.589	2007.044	4542.724	396.767	3885.081	-40.586

3.354. Naphtho[2,1,8-*uva*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 121159-18-0
Point Group: C₁

Length: 16.28 Å
Width: 10.48 Å
Breadth: 5.002 Å
L/B Ratio: 1.554

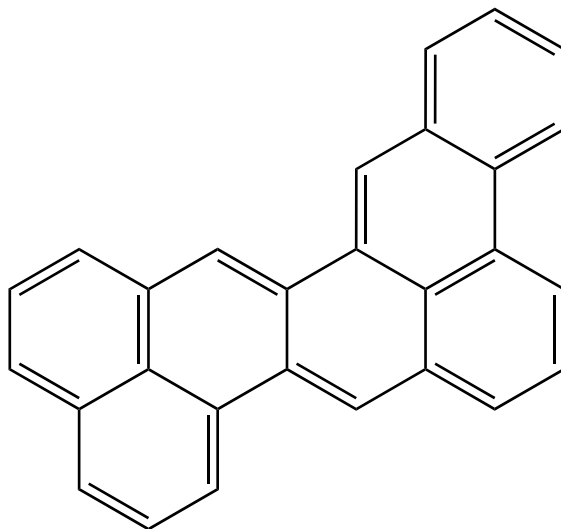
Cartesian coordinates:

C	-5.3208	2.5792	0.5340	C	2.4426	-1.7632	0.2289	H	-6.5633	-0.4898	-0.3250
C	-6.2624	1.5667	0.2090	C	3.8014	-2.1645	0.5050	H	-3.2531	3.0785	0.8074
C	-5.8453	0.2999	-0.0770	C	4.8048	-1.2620	0.5270	H	-4.7191	-2.1244	-0.4900
C	-3.9853	2.3022	0.5578	C	4.5507	0.1314	0.2532	H	-1.4418	1.4961	0.5038
C	-3.5160	0.9887	0.2529	C	5.5839	1.0685	0.2529	H	-2.9652	-3.7531	-0.5720
C	-4.4550	-0.0208	-0.0554	C	5.3208	2.4063	-0.0317	H	-0.5829	-4.3538	-0.2207
C	-3.9915	-1.3247	-0.3022	C	4.0326	2.8245	-0.3267	H	1.6483	-3.7654	0.2547
C	-2.1410	0.6875	0.2454	C	3.2266	0.5481	-0.0265	H	3.9912	-3.2266	0.6987
C	-1.6689	-0.5791	-0.0703	C	2.9774	1.9028	-0.3303	H	5.8357	-1.5642	0.7441
C	-2.6352	-1.6115	-0.2797	C	1.6361	2.2906	-0.6610	H	6.6080	0.7483	0.4757
C	-2.2059	-2.9846	-0.3867	C	0.6197	1.3979	-0.6113	H	6.1412	3.1317	-0.0263
C	-0.9110	-3.3076	-0.2097	C	0.8140	0.0244	-0.2234	H	3.8323	3.8764	-0.5593
C	-0.2472	-0.9182	-0.1147	C	2.1455	-0.3959	-0.0057	H	1.4585	3.3276	-0.9692
C	0.0944	-2.2851	-0.0412	H	-5.6864	3.5852	0.7645	H	-0.3900	1.7218	-0.8996
C	1.4217	-2.6962	0.1553	H	-7.3272	1.8210	0.1948				

Table 3.354: Table of thermodynamic data as a function of temperature for Naphtho[2,1,8-*uva*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-51.470	467.410	467.410	∞
100	110.308	354.061	800.750	-44.669	494.234	542.075	-283.145
200	223.607	463.358	604.625	-28.253	479.969	595.616	-155.556
250	288.996	520.234	582.028	-15.448	473.318	625.298	-130.646
298.15	352.493	576.581	576.581	0.000	467.410	655.119	-114.772
300	354.900	578.769	576.588	0.654	467.193	656.283	-114.267
350	418.157	638.277	581.143	19.997	461.755	688.240	-102.712
400	476.785	697.999	592.019	42.392	457.039	720.916	-94.140
450	529.896	757.279	607.094	67.583	452.957	754.150	-87.538
500	577.379	815.615	625.039	95.288	449.422	787.831	-82.302
600	657.032	928.212	666.268	157.167	443.685	856.082	-74.527
700	720.042	1034.411	711.354	226.140	439.511	925.171	-69.036
800	770.578	1133.977	758.027	300.760	436.719	994.747	-64.949
900	811.753	1227.195	805.035	379.945	435.131	1064.592	-61.786
1000	845.756	1314.537	851.665	462.873	434.583	1134.570	-59.263
1100	874.139	1396.517	897.509	548.909	434.875	1204.570	-57.199
1200	898.036	1473.631	942.338	637.551	435.866	1274.494	-55.476
1300	918.302	1546.334	986.030	728.395	437.370	1344.325	-54.015
1400	935.599	1615.037	1028.528	821.113	439.255	1414.029	-52.757
1500	950.446	1680.106	1069.817	915.434	441.440	1483.589	-51.662
1600	963.260	1741.865	1109.907	1011.134	443.793	1552.987	-50.699
1700	974.376	1800.604	1148.822	1108.029	446.240	1622.211	-49.843
1800	984.066	1856.578	1186.600	1205.962	448.704	1691.355	-49.081
1900	992.552	1910.016	1223.279	1304.802	451.157	1760.309	-48.393
2000	1000.016	1961.122	1258.902	1404.438	453.541	1829.162	-47.772
2100	1006.610	2010.075	1293.515	1504.776	455.779	1897.884	-47.206
2200	1012.459	2057.041	1327.161	1605.736	457.870	1966.506	-46.690
2300	1017.667	2102.163	1359.882	1707.247	459.809	2035.035	-46.216
2400	1022.320	2145.575	1391.720	1809.250	461.525	2103.435	-45.779
2500	1026.493	2187.394	1422.716	1911.695	463.029	2171.884	-45.378
2600	1030.248	2227.728	1452.907	2014.535	464.286	2240.158	-45.004
2700	1033.637	2266.675	1482.330	2117.732	465.299	2308.462	-44.659
2800	1036.705	2304.322	1511.018	2221.252	466.042	2376.756	-44.338
2900	1039.490	2340.751	1539.005	2325.064	466.486	2444.974	-44.038
3000	1042.025	2376.035	1566.321	2429.141	466.676	2513.208	-43.758
3100	1044.339	2410.241	1592.995	2533.461	466.532	2581.362	-43.495
3200	1046.456	2443.431	1619.055	2638.003	466.097	2649.601	-43.249
3300	1048.398	2475.662	1644.527	2742.747	465.353	2717.899	-43.020
3400	1050.183	2506.987	1669.435	2847.677	464.272	2786.135	-42.803
3500	1051.827	2537.453	1693.802	2952.779	462.857	2854.389	-42.599
3600	1053.344	2567.106	1717.651	3058.038	461.133	2922.778	-42.408
3700	1054.747	2595.986	1741.001	3163.444	459.066	2991.237	-42.228
3800	1056.047	2624.131	1763.872	3268.984	456.631	3059.694	-42.058
3900	1057.254	2651.578	1786.284	3374.650	453.869	3128.167	-41.896
4000	1058.376	2678.360	1808.252	3480.432	450.763	3196.858	-41.746
4100	1059.421	2704.507	1829.794	3586.323	447.277	3265.555	-41.603
4200	1060.395	2730.048	1850.926	3692.314	443.441	3334.332	-41.468
4300	1061.306	2755.011	1871.662	3798.400	439.238	3403.112	-41.339
4400	1062.157	2779.420	1892.017	3904.573	434.680	3472.089	-41.218
4500	1062.955	2803.298	1912.003	4010.829	429.780	3541.231	-41.105
4600	1063.703	2826.669	1931.634	4117.163	424.485	3610.494	-40.998
4700	1064.406	2849.553	1950.922	4223.568	418.811	3679.760	-40.895
4800	1065.067	2871.969	1969.877	4330.042	412.805	3749.259	-40.799
4900	1065.690	2893.937	1988.512	4436.581	406.391	3818.747	-40.707
5000	1066.276	2915.473	2006.837	4543.179	399.666	3888.562	-40.623

3.355. Dibenzo[*de,ij*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-46-3
Point Group: C_s

Length: 15.96 Å
Width: 10.41 Å
Breadth: 3.889 Å
L/B Ratio: 1.533

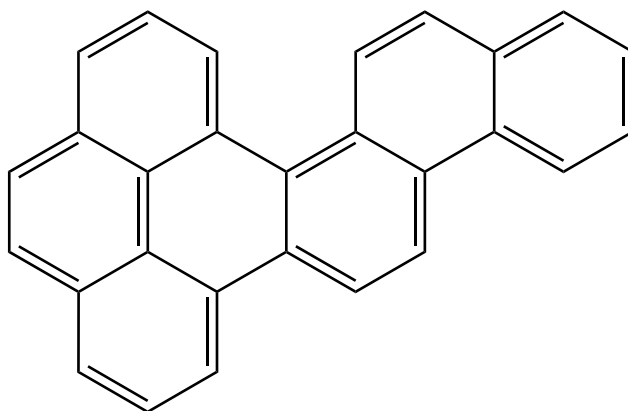
Cartesian coordinates:

C	3.8273	2.7228	0.0000	C	-3.3505	0.3076	0.0000	H	-2.7813	3.6879	0.0000
C	3.1119	1.5048	0.0000	C	-2.6356	1.5400	0.0000	H	-0.6518	2.4674	0.0000
C	3.8148	0.2874	0.0000	C	-1.1907	1.5055	0.0000	H	-1.0406	-3.0695	0.0000
C	5.2257	0.3086	0.0000	C	-4.7607	0.3248	0.0000	H	1.0650	-4.2978	0.0000
C	5.9076	1.5038	0.0000	C	-5.4406	1.5702	0.0000	H	3.5475	-4.3382	0.0000
C	5.2034	2.7196	0.0000	C	-4.7336	2.7455	0.0000	H	4.8384	-2.2042	0.0000
C	3.0748	-0.9550	0.0000	C	-3.3252	2.7365	0.0000	H	-6.5680	-0.8836	0.0000
C	1.6676	-0.9250	0.0000	C	3.7375	-2.1980	0.0000	H	-5.3342	-3.0441	0.0000
C	0.9681	0.3360	0.0000	C	3.0223	-3.3774	0.0000	H	-2.8497	-3.0760	0.0000
C	1.6806	1.5021	0.0000	C	1.6243	-3.3553	0.0000	H	1.1503	2.4685	0.0000
C	0.9454	-2.1434	0.0000	C	-3.3818	-2.1121	0.0000	H	5.7627	-0.6524	0.0000
C	-0.4992	-2.1089	0.0000	C	-4.7918	-2.0928	0.0000	H	7.0024	1.5146	0.0000
C	-1.1920	-0.9441	0.0000	C	-5.4724	-0.9047	0.0000	H	5.7584	3.6634	0.0000
C	-0.4966	0.3405	0.0000	H	-5.2588	3.7065	0.0000	H	3.2732	3.6683	0.0000
C	-2.6559	-0.9384	0.0000	H	-6.5365	1.5758	0.0000				

Table 3.355: Table of thermodynamic data as a function of temperature for Dibenzo[de,ij]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-52.060	497.816	497.816	∞
100	113.824	360.763	811.097	-45.033	524.275	571.446	-298.486
200	225.276	472.031	613.755	-28.345	510.283	624.195	-163.020
250	289.863	529.186	591.098	-15.478	503.694	653.436	-136.525
298.15	352.905	585.643	585.643	0.000	497.816	682.823	-119.625
300	355.300	587.833	585.649	0.655	497.599	683.970	-119.087
350	418.309	647.382	590.208	20.011	492.175	715.473	-106.776
400	476.812	707.116	601.090	42.410	487.462	747.693	-97.637
450	529.861	766.394	616.171	67.601	483.381	780.472	-90.593
500	577.315	824.725	634.119	95.303	479.843	813.697	-85.005
600	656.942	937.308	675.352	157.174	474.098	881.037	-76.700
700	719.938	1043.491	720.438	226.137	469.913	949.218	-70.830
800	770.461	1143.043	767.110	300.747	467.111	1017.886	-66.460
900	811.626	1236.247	814.115	379.919	465.511	1086.825	-63.076
1000	845.623	1323.575	860.741	462.834	464.950	1155.899	-60.377
1100	874.002	1405.542	906.581	548.856	465.229	1224.997	-58.169
1200	897.900	1482.644	951.406	637.485	466.205	1294.018	-56.326
1300	918.168	1555.336	995.093	728.316	467.696	1362.948	-54.763
1400	935.468	1624.029	1037.587	821.020	469.568	1431.752	-53.418
1500	950.320	1689.089	1078.871	915.328	471.740	1500.414	-52.248
1600	963.140	1750.841	1118.956	1011.016	474.080	1568.914	-51.219
1700	974.261	1809.572	1157.867	1107.899	476.515	1637.241	-50.305
1800	983.957	1865.540	1195.640	1205.821	478.969	1705.489	-49.491
1900	992.449	1918.973	1232.314	1304.650	481.411	1773.546	-48.757
2000	999.919	1970.072	1267.934	1404.277	483.785	1841.504	-48.094
2100	1006.519	2019.022	1302.543	1504.605	486.013	1909.331	-47.491
2200	1012.373	2065.983	1336.185	1605.556	488.096	1977.059	-46.940
2300	1017.585	2111.102	1368.902	1707.059	490.027	2044.694	-46.436
2400	1022.243	2154.510	1400.737	1809.054	491.734	2112.200	-45.970
2500	1026.421	2196.326	1431.730	1911.491	493.231	2179.756	-45.543
2600	1030.179	2236.658	1461.917	2014.324	494.481	2247.136	-45.145
2700	1033.572	2275.602	1491.337	2117.515	495.487	2314.548	-44.777
2800	1036.643	2313.247	1520.022	2221.028	496.224	2381.950	-44.435
2900	1039.432	2349.673	1548.006	2324.834	496.662	2449.275	-44.115
3000	1041.970	2384.955	1575.320	2428.906	496.846	2516.617	-43.817
3100	1044.287	2419.159	1601.991	2533.221	496.697	2583.879	-43.537
3200	1046.407	2452.348	1628.049	2637.757	496.257	2651.226	-43.276
3300	1048.351	2484.578	1653.518	2742.496	495.509	2718.633	-43.031
3400	1050.138	2515.901	1678.424	2847.422	494.422	2785.977	-42.800
3500	1051.784	2546.366	1702.789	2952.519	493.003	2853.339	-42.583
3600	1053.304	2576.018	1726.636	3057.775	491.275	2920.837	-42.379
3700	1054.709	2604.896	1749.984	3163.176	489.204	2988.405	-42.188
3800	1056.010	2633.041	1772.854	3268.713	486.765	3055.971	-42.006
3900	1057.219	2660.487	1795.263	3374.375	483.999	3123.553	-41.834
4000	1058.342	2687.268	1817.230	3480.154	480.890	3191.354	-41.674
4100	1059.389	2713.414	1838.770	3586.041	477.401	3259.159	-41.521
4200	1060.364	2738.955	1859.900	3692.029	473.561	3327.046	-41.377
4300	1061.276	2763.917	1880.635	3798.112	469.356	3394.936	-41.239
4400	1062.129	2788.325	1900.988	3904.283	464.795	3463.022	-41.110
4500	1062.928	2812.203	1920.973	4010.536	459.892	3531.273	-40.989
4600	1063.677	2835.573	1940.602	4116.866	454.595	3599.646	-40.874
4700	1064.381	2858.456	1959.888	4223.270	448.918	3668.021	-40.765
4800	1065.043	2880.872	1978.843	4329.741	442.909	3736.630	-40.662
4900	1065.666	2902.839	1997.476	4436.277	436.493	3805.228	-40.563
5000	1066.254	2924.374	2015.800	4542.873	429.765	3874.153	-40.472

3.356. Naphtho[2,1,8-*def*]picene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-39-4
Point Group: C₁

Length: 15.90 Å
Width: 10.46 Å
Breadth: 4.936 Å
L/B Ratio: 1.521

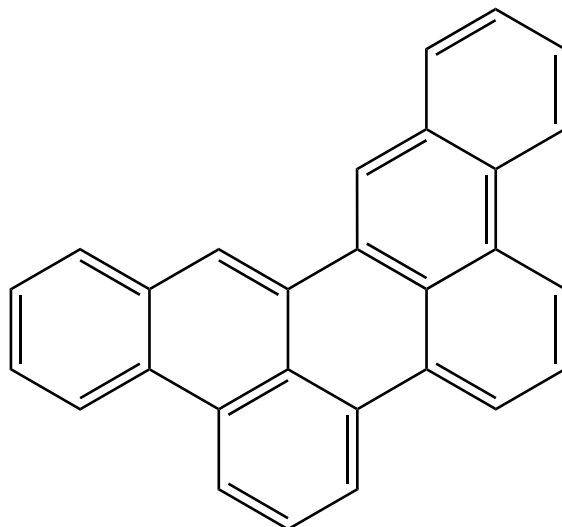
Cartesian coordinates:

C	2.9703	3.2193	-0.3007	C	0.4778	-1.2211	-0.1674	H	1.3406	4.5204	-0.8261
C	0.6832	2.4908	-0.5270	C	-0.4486	-2.2788	-0.3326	H	5.4614	2.4026	0.2361
C	1.6445	3.4989	-0.5736	C	-1.7924	-2.0369	-0.3655	H	6.1961	0.0468	0.5228
C	3.3588	1.8971	-0.0443	C	-1.3817	0.3265	0.0720	H	5.6825	-2.3463	0.4653
C	4.7426	1.5763	0.1895	C	-2.2856	-0.7342	-0.1218	H	4.0310	-4.1882	0.2243
C	5.1437	0.2943	0.3428	C	-3.2549	1.7924	0.6398	H	1.6278	-3.6857	-0.1108
C	4.1972	-0.7857	0.2548	C	-1.9221	1.5829	0.5132	H	-0.0663	-3.3050	-0.4440
C	4.6203	-2.1207	0.3181	C	-4.1931	0.7574	0.3271	H	-2.5107	-2.8514	-0.5447
C	3.6992	-3.1453	0.1843	C	-3.7119	-0.5095	-0.0417	H	-3.6407	2.7564	0.9914
C	2.3484	-2.8612	-0.0016	C	-4.6438	-1.5338	-0.3260	H	-1.2268	2.3920	0.7758
C	2.3914	0.8692	-0.0372	C	-5.9954	-1.2929	-0.2527	H	-4.2643	-2.5278	-0.6074
C	2.8282	-0.4928	0.0771	C	-6.4708	-0.0208	0.1118	H	-6.7111	-2.0903	-0.4778
C	1.8926	-1.5433	-0.0454	C	-5.5845	0.9901	0.4001	H	-7.5500	0.1560	0.1646
C	1.0149	1.1758	-0.1988	H	3.7209	4.0174	-0.3047	H	-5.9450	1.9839	0.6885
C	0.0257	0.1026	-0.0942	H	-0.3584	2.7573	-0.7528				

Table 3.356: Table of thermodynamic data as a function of temperature for Naphtho[2,1,8-*def*]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-51.554	460.830	460.830	∞
100	111.370	354.293	801.265	-44.697	487.625	535.443	-279.681
200	223.662	464.043	605.154	-28.222	473.420	588.930	-153.810
250	288.642	520.883	582.586	-15.426	466.761	618.578	-129.242
298.15	351.933	577.147	577.147	0.000	460.830	648.370	-113.589
300	354.336	579.332	577.154	0.653	460.612	649.532	-113.091
350	417.529	638.747	581.702	19.966	455.144	681.464	-101.701
400	476.174	698.386	592.561	42.330	450.396	714.119	-93.252
450	529.333	757.596	607.616	67.491	446.285	747.335	-86.747
500	576.872	815.875	625.537	95.169	442.723	781.002	-81.589
600	656.607	928.388	666.719	157.002	436.940	849.231	-73.931
700	719.656	1034.525	711.761	225.935	432.725	918.306	-68.523
800	770.203	1134.041	758.394	300.517	429.896	987.873	-64.500
900	811.377	1227.214	805.366	379.664	428.270	1057.714	-61.387
1000	845.379	1314.517	851.962	462.554	427.685	1127.692	-58.903
1100	873.765	1396.461	897.776	548.553	427.939	1197.697	-56.873
1200	897.669	1473.542	942.577	637.158	428.893	1267.627	-55.177
1300	917.945	1546.217	986.243	727.966	430.360	1337.469	-53.739
1400	935.254	1614.894	1028.716	820.648	432.211	1407.185	-52.502
1500	950.116	1679.939	1069.982	914.936	434.362	1476.761	-51.424
1600	962.946	1741.678	1110.050	1010.604	436.682	1546.177	-50.476
1700	974.079	1800.398	1148.946	1107.468	439.099	1615.421	-49.635
1800	983.784	1856.356	1186.704	1205.372	441.535	1684.587	-48.884
1900	992.286	1909.779	1223.366	1304.185	443.959	1753.563	-48.208
2000	999.766	1960.871	1258.973	1403.796	446.318	1822.441	-47.596
2100	1006.375	2009.813	1293.570	1504.109	448.532	1891.188	-47.040
2200	1012.237	2056.767	1327.201	1605.046	450.600	1959.837	-46.531
2300	1017.457	2101.880	1359.908	1706.535	452.518	2028.394	-46.065
2400	1022.123	2145.283	1391.734	1808.519	454.213	2096.823	-45.635
2500	1026.307	2187.095	1422.717	1910.944	455.698	2165.301	-45.241
2600	1030.072	2227.422	1452.896	2013.766	456.936	2233.605	-44.873
2700	1033.471	2266.362	1482.308	2116.946	457.932	2301.941	-44.533
2800	1036.548	2304.003	1510.986	2220.449	458.660	2370.267	-44.217
2900	1039.341	2340.427	1538.962	2324.246	459.088	2438.517	-43.922
3000	1041.884	2375.705	1566.269	2428.309	459.264	2506.783	-43.646
3100	1044.206	2409.907	1592.934	2532.616	459.106	2574.971	-43.387
3200	1046.330	2443.093	1618.986	2637.144	458.658	2643.243	-43.146
3300	1048.278	2475.321	1644.449	2741.876	457.902	2711.575	-42.920
3400	1050.068	2506.642	1669.350	2846.794	456.809	2779.845	-42.706
3500	1051.718	2537.105	1693.709	2951.885	455.383	2848.134	-42.505
3600	1053.240	2566.754	1717.551	3057.134	453.648	2916.558	-42.317
3700	1054.648	2595.632	1740.894	3162.529	451.571	2985.052	-42.141
3800	1055.953	2623.775	1763.759	3268.060	449.126	3053.545	-41.973
3900	1057.164	2651.219	1786.164	3373.716	446.355	3122.053	-41.814
4000	1058.290	2677.999	1808.126	3479.490	443.240	3190.781	-41.666
4100	1059.338	2704.144	1829.663	3585.372	439.746	3259.513	-41.526
4200	1060.316	2729.683	1850.789	3691.355	435.901	3328.327	-41.393
4300	1061.230	2754.644	1871.520	3797.433	431.691	3397.144	-41.266
4400	1062.085	2779.051	1891.869	3903.599	427.125	3466.158	-41.148
4500	1062.885	2802.928	1911.851	4009.848	422.218	3535.336	-41.036
4600	1063.636	2826.297	1931.477	4116.174	416.917	3604.637	-40.931
4700	1064.342	2849.180	1950.760	4222.574	411.236	3673.940	-40.830
4800	1065.005	2871.595	1969.711	4329.041	405.224	3743.476	-40.736
4900	1065.630	2893.561	1988.342	4435.573	398.804	3813.002	-40.646
5000	1066.219	2915.096	2006.662	4542.166	392.072	3882.855	-40.563

3.357. Dibenzo[*fg,ij*]pentaphene



Other names: Dibenzo[*b,n*]perylene
2,3,10,11-Dibenzoperylene

Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 197-69-3
Point Group: C_{2v}

Length: 15.90 Å
Width: 10.44 Å
Breadth: 3.885 Å
L/B Ratio: 1.524

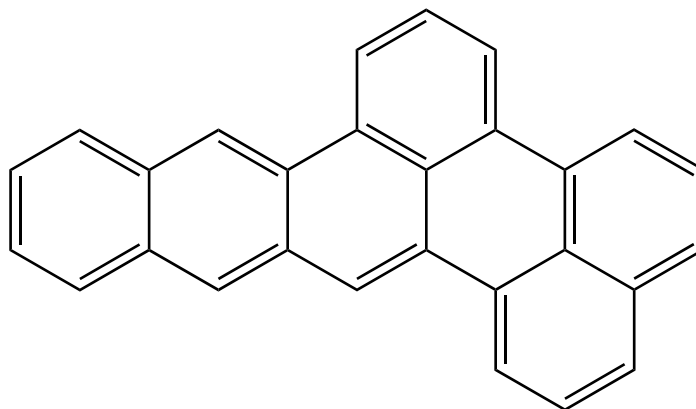
Cartesian coordinates:

C	3.5664	2.8709	0.0000	C	-3.5753	0.4372	0.0000	H	-5.5361	-0.4797	0.0000
C	2.8635	1.6454	0.0000	C	-2.8622	1.6476	0.0000	H	-2.9995	3.8129	0.0000
C	3.5757	0.4344	0.0000	C	-1.4319	1.6279	0.0000	H	-0.8939	2.5900	0.0000
C	4.9870	0.4702	0.0000	C	-4.9865	0.4741	0.0000	H	0.8886	-4.1817	0.0000
C	5.6573	1.6716	0.0000	C	-5.6560	1.6761	0.0000	H	3.3723	-4.1887	0.0000
C	4.9421	2.8812	0.0000	C	-4.9398	2.8851	0.0000	H	4.6323	-2.0352	0.0000
C	2.8456	-0.8142	0.0000	C	-3.5641	2.8737	0.0000	H	0.8960	2.5893	0.0000
C	1.4370	-0.8038	0.0000	C	3.5315	-2.0458	0.0000	H	-4.6339	-2.0313	0.0000
C	0.7321	0.4546	0.0000	C	2.8364	-3.2340	0.0000	H	-3.3757	-4.1860	0.0000
C	1.4332	1.6267	0.0000	C	1.4378	-3.2277	0.0000	H	-0.8919	-4.1810	0.0000
C	0.7308	-2.0333	0.0000	C	-1.4404	-3.2266	0.0000	H	5.5358	-0.4840	0.0000
C	-0.7324	-2.0327	0.0000	C	-2.8390	-3.2317	0.0000	H	6.7520	1.6928	0.0000
C	-1.4376	-0.8027	0.0000	C	-3.5332	-2.0429	0.0000	H	5.4884	3.8300	0.0000
C	-0.7317	0.4551	0.0000	H	-5.4854	3.8343	0.0000	H	3.0025	3.8105	0.0000
C	-2.8463	-0.8119	0.0000	H	-6.7506	1.6981	0.0000				

Table 3.357: Table of thermodynamic data as a function of temperature for Dibenzo[fg,ij]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-52.094	459.745	459.745	∞
100	114.556	358.183	807.641	-44.946	486.291	533.720	-278.781
200	224.722	469.566	610.807	-28.248	472.308	586.714	-153.231
250	288.835	526.543	588.230	-15.422	465.679	616.081	-128.720
298.15	351.626	582.794	582.794	0.000	459.745	645.601	-113.104
300	354.014	584.977	582.801	0.653	459.525	646.753	-112.607
350	416.930	644.319	587.344	19.941	454.034	678.404	-101.244
400	475.439	703.868	598.189	42.272	449.252	710.782	-92.817
450	528.544	762.988	613.222	67.395	445.103	743.727	-86.328
500	576.075	821.183	631.118	95.033	441.501	777.126	-81.184
600	655.861	933.555	672.242	156.788	435.640	844.831	-73.548
700	718.989	1039.582	717.224	225.650	431.355	913.396	-68.157
800	769.616	1139.014	763.802	300.170	428.463	982.461	-64.147
900	810.862	1232.123	810.721	379.262	426.782	1051.808	-61.044
1000	844.926	1319.374	857.271	462.104	426.148	1121.298	-58.569
1100	873.365	1401.278	903.041	548.060	426.361	1190.819	-56.546
1200	897.313	1478.326	947.804	636.627	427.276	1260.270	-54.857
1300	917.629	1550.974	991.434	727.402	428.710	1329.634	-53.424
1400	934.971	1619.629	1033.876	820.054	430.531	1398.876	-52.192
1500	949.862	1684.656	1075.113	914.314	432.655	1467.980	-51.119
1600	962.716	1746.379	1115.154	1009.959	434.951	1536.925	-50.174
1700	973.870	1805.085	1154.026	1106.801	437.346	1605.699	-49.336
1800	983.595	1861.032	1191.762	1204.685	439.762	1674.396	-48.589
1900	992.113	1914.445	1228.403	1303.480	442.168	1742.906	-47.915
2000	999.607	1965.529	1263.992	1403.074	444.510	1811.317	-47.306
2100	1006.229	2014.463	1298.572	1503.372	446.709	1879.599	-46.752
2200	1012.102	2061.411	1332.186	1604.294	448.763	1947.783	-46.245
2300	1017.333	2106.518	1364.879	1705.771	450.668	2015.876	-45.781
2400	1022.007	2149.916	1396.690	1807.743	452.351	2083.841	-45.353
2500	1026.200	2191.723	1427.661	1910.157	453.825	2151.857	-44.960
2600	1029.972	2232.046	1457.828	2012.969	455.053	2219.698	-44.593
2700	1033.378	2270.983	1487.228	2116.139	456.039	2287.572	-44.255
2800	1036.460	2308.621	1515.895	2219.633	456.758	2355.435	-43.940
2900	1039.259	2345.041	1543.861	2323.421	457.178	2423.224	-43.646
3000	1041.808	2380.317	1571.158	2427.477	457.345	2491.029	-43.372
3100	1044.134	2414.517	1597.815	2531.776	457.180	2558.755	-43.114
3200	1046.262	2447.701	1623.858	2636.297	456.726	2626.567	-42.873
3300	1048.214	2479.926	1649.313	2741.022	455.963	2694.438	-42.649
3400	1050.008	2511.245	1674.206	2845.934	454.863	2762.248	-42.436
3500	1051.660	2541.707	1698.558	2951.019	453.432	2830.076	-42.236
3600	1053.186	2571.355	1722.393	3056.262	451.691	2898.040	-42.049
3700	1054.597	2600.230	1745.730	3161.652	449.609	2966.074	-41.873
3800	1055.904	2628.372	1768.588	3267.178	447.159	3034.107	-41.706
3900	1057.117	2655.816	1790.987	3372.830	444.383	3102.156	-41.548
4000	1058.245	2682.594	1812.944	3478.599	441.263	3170.424	-41.401
4100	1059.296	2708.738	1834.475	3584.476	437.765	3238.697	-41.261
4200	1060.276	2734.276	1855.596	3690.455	433.916	3307.052	-41.128
4300	1061.191	2759.236	1876.322	3796.529	429.702	3375.409	-41.002
4400	1062.047	2783.642	1896.667	3902.692	425.132	3443.964	-40.884
4500	1062.850	2807.518	1916.643	4008.937	420.222	3512.684	-40.773
4600	1063.602	2830.887	1936.265	4115.260	414.917	3581.525	-40.669
4700	1064.309	2853.769	1955.544	4221.656	409.233	3650.369	-40.568
4800	1064.974	2876.183	1974.491	4328.120	403.217	3719.446	-40.475
4900	1065.600	2898.148	1993.118	4434.649	396.794	3788.513	-40.385
5000	1066.190	2919.682	2011.435	4541.239	390.060	3857.908	-40.302

3.358. Dibenzo[*de, st*]pentacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 14147-38-7
Point Group: C_s

Length: 16.74 Å
Width: 10.81 Å
Breadth: 3.887 Å
L/B Ratio: 1.549

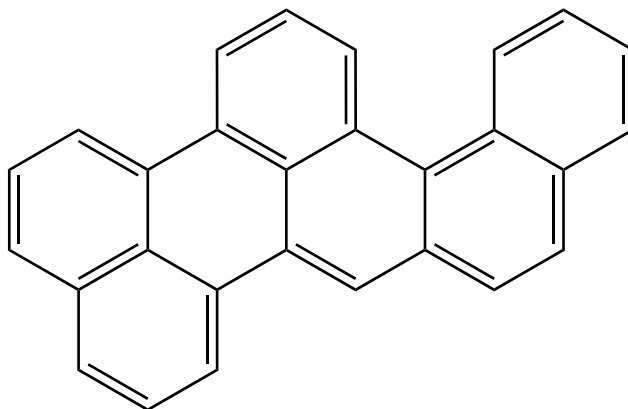
Cartesian coordinates:

C	2.1848	2.6640	0.0000	C	0.4424	-3.5822	0.0000	H	3.5248	4.3632	0.0000
C	4.5898	2.5020	0.0000	C	1.6955	-2.9702	0.0000	H	4.2181	-2.8016	0.0000
C	3.4571	3.2703	0.0000	C	1.8106	-1.5835	0.0000	H	6.4495	-1.7155	0.0000
C	4.4911	1.0849	0.0000	C	-1.8308	-0.6015	0.0000	H	6.6410	0.7654	0.0000
C	4.2859	-1.7028	0.0000	C	-1.7119	0.8163	0.0000	H	-0.3327	2.5128	0.0000
C	5.5529	-1.0870	0.0000	C	-2.8504	1.6111	0.0000	H	-1.6971	-3.2829	0.0000
C	5.6593	0.2783	0.0000	C	-3.0923	-1.1784	0.0000	H	0.3714	-4.6748	0.0000
C	3.2192	0.4729	0.0000	C	-4.2514	-0.3825	0.0000	H	2.6085	-3.5853	0.0000
C	2.0503	1.2907	0.0000	C	-4.1294	1.0277	0.0000	H	-2.7580	2.7042	0.0000
C	3.1291	-0.9504	0.0000	C	-5.3125	1.8276	0.0000	H	-3.1839	-2.2765	0.0000
C	0.7301	0.6602	0.0000	C	-6.5425	1.2389	0.0000	H	-5.2088	2.9185	0.0000
C	-0.4039	1.4126	0.0000	C	-6.6648	-0.1765	0.0000	H	-7.4529	1.8472	0.0000
C	0.6426	-0.7860	0.0000	C	-5.5539	-0.9675	0.0000	H	-7.6660	-0.6197	0.0000
C	-0.6207	-1.4077	0.0000	H	1.2836	3.2965	0.0000	H	-5.6390	-2.0600	0.0000
C	-0.7025	-2.8110	0.0000	H	5.5832	2.9646	0.0000				

Table 3.358: Table of thermodynamic data as a function of temperature for Dibenzo[de,si]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-52.231	468.512	468.512	∞
100	114.291	372.693	822.442	-44.975	495.029	541.007	-282.587
200	224.890	483.945	625.413	-28.294	481.030	592.560	-154.758
250	289.326	540.996	602.796	-15.450	474.418	621.207	-129.791
298.15	352.286	597.351	597.351	0.000	468.512	650.028	-113.880
300	354.679	599.537	597.357	0.654	468.294	651.153	-113.373
350	417.651	658.987	601.909	19.977	462.837	682.073	-101.792
400	476.149	718.632	612.773	42.344	458.092	713.716	-93.200
450	529.213	777.834	627.831	67.501	453.977	745.920	-86.582
500	576.693	836.097	645.754	95.172	450.408	778.575	-81.336
600	656.383	948.572	686.933	156.983	444.603	844.784	-73.543
700	719.439	1054.674	731.968	225.894	440.366	911.843	-68.041
800	770.014	1154.163	778.592	300.456	437.516	979.396	-63.947
900	811.222	1247.316	825.554	379.586	435.874	1047.225	-60.778
1000	845.255	1334.604	872.142	462.462	435.274	1115.194	-58.251
1100	873.668	1416.538	917.947	548.450	435.518	1183.191	-56.184
1200	897.594	1493.612	962.739	637.047	436.463	1251.114	-54.458
1300	917.889	1566.281	1006.397	727.848	437.924	1318.949	-52.995
1400	935.212	1634.954	1048.864	820.526	439.769	1386.659	-51.736
1500	950.085	1699.997	1090.124	914.809	441.917	1454.229	-50.640
1600	962.924	1761.734	1130.187	1010.475	444.235	1521.640	-49.675
1700	974.062	1820.453	1169.078	1107.337	446.649	1588.878	-48.819
1800	983.773	1876.410	1206.832	1205.240	449.084	1656.038	-48.056
1900	992.279	1929.833	1243.490	1304.052	451.508	1723.009	-47.368
2000	999.762	1980.924	1279.093	1403.661	453.865	1789.881	-46.746
2100	1006.373	2029.866	1313.687	1503.975	456.079	1856.624	-46.180
2200	1012.237	2076.820	1347.315	1604.911	458.147	1923.267	-45.663
2300	1017.459	2121.934	1380.020	1706.401	460.065	1989.819	-45.189
2400	1022.125	2165.337	1411.843	1808.384	461.760	2056.242	-44.752
2500	1026.310	2207.148	1442.824	1910.810	463.246	2122.715	-44.351
2600	1030.076	2247.475	1473.001	2013.632	464.484	2189.014	-43.977
2700	1033.475	2286.416	1502.411	2116.813	465.481	2255.344	-43.631
2800	1036.552	2324.057	1531.087	2220.317	466.209	2321.665	-43.310
2900	1039.346	2360.481	1559.062	2324.114	466.638	2387.909	-43.010
3000	1041.889	2395.760	1586.367	2428.178	466.813	2454.171	-42.730
3100	1044.211	2429.961	1613.031	2532.484	466.656	2520.352	-42.467
3200	1046.335	2463.148	1639.081	2637.013	466.209	2586.619	-42.221
3300	1048.283	2495.376	1664.544	2741.745	465.453	2652.946	-41.992
3400	1050.073	2526.697	1689.443	2846.664	464.360	2719.210	-41.775
3500	1051.723	2557.160	1713.801	2951.755	462.935	2785.493	-41.570
3600	1053.245	2586.810	1737.642	3057.005	461.201	2851.912	-41.379
3700	1054.653	2615.687	1760.984	3162.401	459.125	2918.400	-41.200
3800	1055.958	2643.830	1783.848	3267.932	456.680	2984.888	-41.029
3900	1057.168	2671.275	1806.252	3373.589	453.909	3051.391	-40.868
4000	1058.294	2698.055	1828.214	3479.363	450.795	3118.113	-40.718
4100	1059.343	2724.200	1849.750	3585.245	447.301	3184.840	-40.575
4200	1060.320	2749.739	1870.875	3691.229	443.457	3251.648	-40.439
4300	1061.234	2774.700	1891.605	3797.307	439.247	3318.459	-40.310
4400	1062.089	2799.107	1911.954	3903.474	434.682	3385.467	-40.190
4500	1062.889	2822.984	1931.935	4009.723	429.775	3452.640	-40.076
4600	1063.640	2846.354	1951.560	4116.050	424.474	3519.935	-39.969
4700	1064.345	2869.236	1970.843	4222.450	418.794	3587.232	-39.867
4800	1065.009	2891.651	1989.793	4328.918	412.782	3654.763	-39.771
4900	1065.633	2913.617	2008.424	4435.450	406.362	3722.283	-39.679
5000	1066.222	2935.152	2026.743	4542.043	399.631	3790.131	-39.594

3.359. Naphtho[2,1-*b*]perylene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-43-0
Point Group: C₁

Length: 16.22 Å
Width: 10.28 Å
Breadth: 4.967 Å
L/B Ratio: 1.577

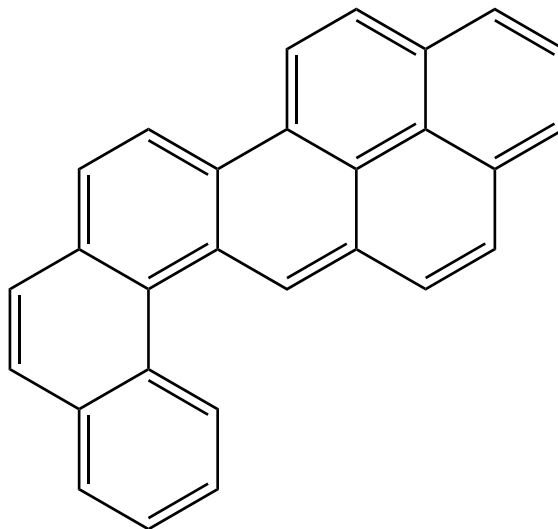
Cartesian coordinates:

C	-5.1316	1.7850	-0.1764	C	-0.7595	-0.8626	0.1018	H	-3.4977	3.2016	0.0389
C	-5.5001	0.4689	-0.2618	C	0.2067	-1.8232	0.2192	H	-5.9408	-2.1820	-0.3948
C	-3.7752	2.1388	-0.0340	C	0.9893	0.8736	0.2141	H	-4.1972	-3.9541	-0.2872
C	-4.5150	-0.5520	-0.2084	C	2.0044	-0.1545	0.1183	H	-1.8006	-3.3443	-0.0491
C	-4.8817	-1.9218	-0.2879	C	1.5885	-1.4837	0.2523	H	2.3527	2.5232	0.6197
C	-3.9214	-2.8960	-0.2296	C	2.5360	-2.5426	0.4220	H	0.6018	4.2422	0.7093
C	-2.5617	-2.5503	-0.0961	C	3.8665	-2.2854	0.4009	H	-1.7870	3.6390	0.3507
C	-2.7901	1.1737	0.0184	C	3.4155	0.0854	-0.1044	H	-0.0835	-2.8862	0.2590
C	-3.1549	-0.2014	-0.0719	C	4.3334	-0.9690	0.0948	H	2.1610	-3.5593	0.5879
C	-2.1690	-1.2296	-0.0214	C	5.7227	-0.7516	-0.0635	H	4.6014	-3.0790	0.5776
C	-1.3794	1.5333	0.1642	C	6.1945	0.4673	-0.4819	H	6.4157	-1.5764	0.1394
C	1.3062	2.2309	0.4578	C	5.2844	1.4973	-0.7767	H	7.2685	0.6397	-0.6050
C	0.3324	3.1982	0.5176	C	3.9361	1.3090	-0.5935	H	5.6595	2.4519	-1.1603
C	-1.0129	2.8565	0.3380	H	-5.8858	2.5779	-0.2165	H	3.2482	2.1262	-0.8495
C	-0.3794	0.5214	0.1426	H	-6.5530	0.1858	-0.3713				

Table 3.359: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*b*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-51.781	483.951	483.951	∞
100	112.637	359.456	807.428	-44.797	510.646	557.947	-291.436
200	224.085	469.864	611.027	-28.233	496.530	610.876	-159.541
250	288.717	526.758	588.455	-15.424	489.883	640.231	-133.766
298.15	351.816	583.017	583.017	0.000	483.951	669.741	-117.333
300	354.214	585.201	583.024	0.653	483.732	670.892	-116.810
350	417.310	644.589	587.570	19.956	478.255	702.531	-104.845
400	475.916	704.196	598.424	42.309	473.495	734.894	-95.965
450	529.066	763.375	613.471	67.457	469.372	767.821	-89.125
500	576.610	821.626	631.383	95.122	465.796	801.199	-83.699
600	656.372	934.094	672.545	156.929	459.988	868.856	-75.639
700	719.450	1040.196	717.567	225.840	455.751	937.362	-69.945
800	770.022	1139.686	764.182	300.403	452.902	1006.363	-65.707
900	811.217	1232.840	811.136	379.533	451.260	1075.640	-62.427
1000	845.237	1320.126	857.718	462.408	450.659	1145.057	-59.810
1100	873.637	1402.057	903.518	548.394	450.900	1214.501	-57.671
1200	897.553	1479.128	948.306	636.987	451.841	1283.873	-55.884
1300	917.841	1551.794	991.960	727.783	453.298	1353.156	-54.369
1400	935.160	1620.463	1034.424	820.456	455.139	1422.316	-53.066
1500	950.030	1685.503	1075.680	914.734	457.281	1491.335	-51.932
1600	962.868	1747.236	1115.740	1010.394	459.593	1560.195	-50.934
1700	974.006	1805.952	1154.627	1107.251	462.002	1628.883	-50.048
1800	983.718	1861.905	1192.379	1205.148	464.431	1697.493	-49.259
1900	992.225	1915.325	1229.033	1303.954	466.849	1765.915	-48.547
2000	999.710	1966.414	1264.634	1403.559	469.202	1834.238	-47.904
2100	1006.322	2015.353	1299.226	1503.867	471.410	1902.432	-47.319
2200	1012.189	2062.305	1332.852	1604.799	473.474	1970.526	-46.785
2300	1017.412	2107.416	1365.554	1706.284	475.387	2038.530	-46.296
2400	1022.081	2150.818	1397.375	1808.263	477.077	2106.405	-45.844
2500	1026.268	2192.627	1428.354	1910.684	478.559	2174.330	-45.429
2600	1030.036	2232.953	1458.529	2013.502	479.793	2242.081	-45.043
2700	1033.436	2271.892	1487.937	2116.679	480.786	2309.863	-44.686
2800	1036.515	2309.532	1516.611	2220.179	481.510	2377.636	-44.354
2900	1039.311	2345.954	1544.584	2323.972	481.935	2445.333	-44.044
3000	1041.856	2381.232	1571.888	2428.033	482.108	2513.047	-43.755
3100	1044.179	2415.433	1598.550	2532.336	481.947	2580.682	-43.483
3200	1046.304	2448.618	1624.599	2636.862	481.497	2648.402	-43.230
3300	1048.254	2480.845	1650.060	2741.591	480.738	2716.181	-42.993
3400	1050.046	2512.165	1674.957	2846.507	479.642	2783.899	-42.769
3500	1051.696	2542.628	1699.315	2951.596	478.215	2851.635	-42.557
3600	1053.220	2572.277	1723.154	3056.842	476.477	2919.507	-42.360
3700	1054.629	2601.153	1746.495	3162.236	474.399	2987.449	-42.174
3800	1055.934	2629.296	1769.358	3267.765	471.952	3055.390	-41.998
3900	1057.146	2656.740	1791.761	3373.420	469.178	3123.346	-41.832
4000	1058.273	2683.519	1813.721	3479.191	466.062	3191.521	-41.676
4100	1059.322	2709.664	1835.256	3585.072	462.566	3259.702	-41.528
4200	1060.301	2735.203	1856.380	3691.053	458.720	3327.964	-41.388
4300	1061.215	2760.163	1877.110	3797.130	454.508	3396.229	-41.255
4400	1062.070	2784.570	1897.457	3903.294	449.941	3464.691	-41.130
4500	1062.872	2808.446	1917.437	4009.542	445.033	3533.318	-41.013
4600	1063.623	2831.816	1937.062	4115.867	439.730	3602.066	-40.902
4700	1064.329	2854.698	1956.343	4222.265	434.048	3670.817	-40.796
4800	1064.993	2877.113	1975.293	4328.732	428.034	3739.801	-40.696
4900	1065.618	2899.078	1993.923	4435.262	421.613	3808.775	-40.601
5000	1066.208	2920.613	2012.242	4541.854	414.881	3878.077	-40.513

3.360. Dibenzo[*a,pqr*]picene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-40-7
Point Group: C₁

Length: 16.26 Å
Width: 10.14 Å
Breadth: 5.029 Å
L/B Ratio: 1.603

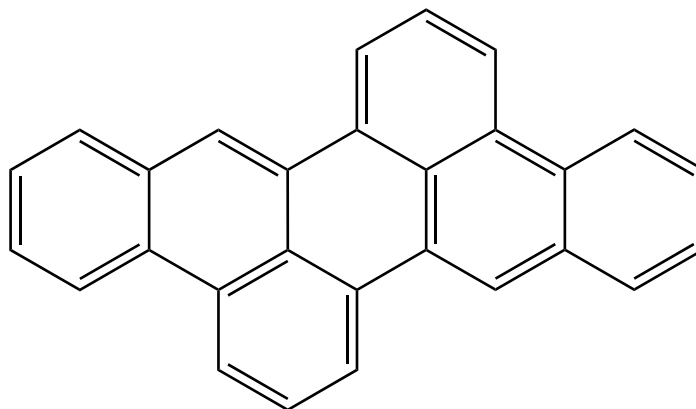
Cartesian coordinates:

C	-5.2788	1.7368	-0.1589	C	-0.0141	-1.4460	0.0654	H	-6.3008	-1.4608	0.4452
C	-6.1310	0.6571	0.0790	C	0.5237	-2.7690	0.0853	H	-4.3601	-2.9881	0.5672
C	-5.6248	-0.6177	0.2636	C	1.8521	-2.9749	-0.0937	H	-1.9066	-3.3499	0.4603
C	-4.2393	-0.8406	0.2177	C	2.2893	-0.5554	-0.0409	H	0.9363	1.7945	-0.4961
C	-3.6766	-2.1494	0.3920	C	2.7512	-1.8690	-0.1826	H	-0.9701	3.2731	-0.7045
C	-2.3358	-2.3439	0.3365	C	4.1342	-2.1464	-0.4184	H	-3.4211	3.6342	-0.6225
C	-1.4266	-1.2529	0.1185	C	5.0418	-1.1403	-0.4572	H	-0.1711	-3.6132	0.2104
C	0.2829	0.9334	-0.2926	C	3.2827	0.4873	0.1203	H	2.2604	-3.9907	-0.1511
C	-3.9009	1.5453	-0.2084	C	4.6382	0.1954	-0.1464	H	4.4386	-3.1863	-0.5855
C	-3.3709	0.2465	-0.0122	C	5.6233	1.2070	-0.0512	H	6.0960	-1.3346	-0.6854
C	-1.9555	0.0326	-0.0519	C	5.2884	2.4687	0.3721	H	6.6612	0.9630	-0.3059
C	-1.0829	1.1318	-0.2871	C	3.9592	2.7461	0.7357	H	6.0473	3.2540	0.4471
C	-1.6566	2.4416	-0.5064	C	2.9879	1.7824	0.6133	H	3.7045	3.7378	1.1242
C	-2.9909	2.6386	-0.4633	H	-5.6963	2.7389	-0.3087	H	1.9621	2.0237	0.9240
C	0.8562	-0.3398	-0.0647	H	-7.2127	0.8243	0.1170				

Table 3.360: Table of thermodynamic data as a function of temperature for Dibenzo[*a,pqr*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-51.422	462.134	462.134	∞
100	110.591	353.173	799.453	-44.628	488.998	536.927	-280.456
200	223.337	462.484	603.553	-28.214	474.732	590.553	-154.234
250	288.577	519.281	580.987	-15.426	468.063	620.281	-129.598
298.15	352.014	575.548	575.548	0.000	462.134	650.150	-113.901
300	354.421	577.733	575.555	0.653	461.915	651.315	-113.402
350	417.678	637.167	580.104	19.972	456.453	683.327	-101.979
400	476.339	696.827	590.967	42.344	451.714	716.059	-93.506
450	529.493	756.057	606.027	67.513	447.611	749.354	-86.981
500	577.018	814.352	623.954	95.199	444.057	783.097	-81.808
600	656.734	926.890	665.148	157.045	438.287	851.477	-74.126
700	719.778	1033.045	710.201	225.991	434.084	920.701	-68.702
800	770.329	1132.578	756.846	300.586	431.267	990.415	-64.666
900	811.511	1225.767	803.828	379.745	429.655	1060.401	-61.543
1000	845.520	1313.084	850.434	462.649	429.083	1130.523	-59.051
1100	873.909	1395.041	896.257	548.662	429.352	1200.671	-57.014
1200	897.814	1472.135	941.067	637.282	430.320	1270.743	-55.313
1300	918.088	1544.821	984.741	728.104	431.802	1340.724	-53.870
1400	935.394	1613.509	1027.222	820.801	433.667	1410.580	-52.628
1500	950.252	1678.564	1068.496	915.102	435.831	1480.294	-51.547
1600	963.076	1740.311	1108.571	1010.784	438.165	1549.847	-50.596
1700	974.202	1799.039	1147.474	1107.660	440.594	1619.226	-49.752
1800	983.902	1855.003	1185.239	1205.577	443.042	1688.528	-48.999
1900	992.398	1908.433	1221.906	1304.401	445.478	1757.639	-48.320
2000	999.872	1959.530	1257.519	1404.022	447.848	1826.651	-47.706
2100	1006.474	2008.477	1292.122	1504.346	450.072	1895.533	-47.148
2200	1012.331	2055.436	1325.758	1605.292	452.150	1964.315	-46.638
2300	1017.546	2100.553	1358.470	1706.791	454.077	2033.005	-46.170
2400	1022.207	2143.960	1390.301	1808.783	455.781	2101.566	-45.738
2500	1026.386	2185.775	1421.288	1911.216	457.274	2170.177	-45.342
2600	1030.147	2226.105	1451.472	2014.046	458.520	2238.612	-44.973
2700	1033.542	2265.048	1480.887	2117.234	459.523	2307.079	-44.632
2800	1036.615	2302.692	1509.569	2220.744	460.258	2375.536	-44.315
2900	1039.405	2339.117	1537.549	2324.547	460.693	2443.917	-44.019
3000	1041.945	2374.398	1564.860	2428.617	460.874	2512.315	-43.742
3100	1044.263	2408.602	1591.528	2532.929	460.722	2580.633	-43.482
3200	1046.384	2441.790	1617.583	2637.463	460.280	2649.036	-43.240
3300	1048.330	2474.019	1643.049	2742.200	459.529	2717.498	-43.014
3400	1050.118	2505.342	1667.953	2847.123	458.441	2785.898	-42.799
3500	1051.765	2535.806	1692.315	2952.219	457.020	2854.316	-42.597
3600	1053.285	2565.457	1716.159	3057.472	455.290	2922.870	-42.409
3700	1054.691	2594.335	1739.505	3162.872	453.217	2991.494	-42.231
3800	1055.994	2622.480	1762.372	3268.407	450.776	3060.117	-42.063
3900	1057.203	2649.925	1784.780	3374.067	448.009	3128.755	-41.904
4000	1058.327	2676.706	1806.745	3479.844	444.898	3197.611	-41.756
4100	1059.374	2702.852	1828.283	3585.730	441.408	3266.473	-41.615
4200	1060.350	2728.392	1849.412	3691.717	437.566	3335.416	-41.481
4300	1061.263	2753.353	1870.144	3797.798	433.360	3404.362	-41.354
4400	1062.116	2777.761	1890.496	3903.967	428.797	3473.505	-41.235
4500	1062.915	2801.639	1910.479	4010.219	423.893	3542.813	-41.123
4600	1063.665	2825.009	1930.107	4116.549	418.594	3612.242	-41.017
4700	1064.370	2847.892	1949.392	4222.951	412.917	3681.674	-40.916
4800	1065.032	2870.307	1968.345	4329.421	406.907	3751.339	-40.822
4900	1065.656	2892.274	1986.977	4435.956	400.490	3820.993	-40.731
5000	1066.243	2913.809	2005.299	4542.551	393.761	3890.975	-40.648

3.361. Dibenzo[fg,qr]pentacene



Other names: Dibenzo[*b,k*]perylene
2,3,8,9-Dibenzoperylene

Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 197-74-0
Point Group: C_{2h}

Length: 16.59 Å
Width: 10.33 Å
Breadth: 3.890 Å
L/B Ratio: 1.606

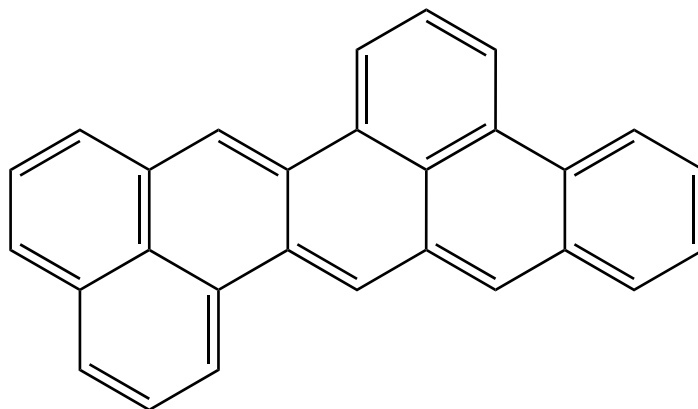
Cartesian coordinates:

C	1.1906	-0.8191	0.0000	C	-2.5692	-1.2241	0.0000	H	1.6202	4.5054	0.0000
C	2.3212	-1.5851	0.0000	C	3.7584	0.4014	0.0000	H	-0.6280	3.4482	0.0000
C	1.2972	0.6193	0.0000	C	3.6249	-0.9971	0.0000	H	-3.6725	-3.0860	0.0000
C	2.5692	1.2241	0.0000	C	4.7803	-1.8106	0.0000	H	-1.6202	-4.5053	0.0000
C	2.6703	2.6308	0.0000	C	6.0312	-1.2384	0.0000	H	0.6280	-3.4482	0.0000
C	1.5385	3.4135	0.0000	C	6.1680	0.1604	0.0000	H	-2.2418	2.6845	0.0000
C	0.2733	2.8162	0.0000	C	5.0527	0.9657	0.0000	H	4.6665	-2.9005	0.0000
C	0.1372	1.4351	0.0000	C	-3.7583	-0.4014	0.0000	H	6.9275	-1.8671	0.0000
C	-0.1372	-1.4350	0.0000	C	-3.6249	0.9971	0.0000	H	7.1690	0.6039	0.0000
C	-2.6703	-2.6307	0.0000	C	-4.7803	1.8105	0.0000	H	5.1467	2.0624	0.0000
C	-1.5385	-3.4135	0.0000	C	-6.0312	1.2383	0.0000	H	-4.6665	2.9005	0.0000
C	-0.2734	-2.8161	0.0000	C	-6.1679	-0.1605	0.0000	H	-6.9275	1.8670	0.0000
C	-1.2972	-0.6192	0.0000	C	-5.0526	-0.9657	0.0000	H	-7.1689	-0.6040	0.0000
C	-1.1906	0.8191	0.0000	H	2.2418	-2.6845	0.0000	H	-5.1465	-2.0624	0.0000
C	-2.3212	1.5851	0.0000	H	3.6725	3.0861	0.0000				

Table 3.361: Table of thermodynamic data as a function of temperature for Dibenzofg,qr]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-52.276	458.173	458.173	∞
100	115.293	362.470	812.518	-45.005	484.660	531.661	-277.705
200	224.969	474.180	615.494	-28.263	470.722	584.205	-152.575
250	288.977	531.199	592.907	-15.427	464.102	613.340	-128.148
298.15	351.702	587.470	587.470	0.000	458.173	642.636	-112.585
300	354.088	589.653	587.476	0.653	457.954	643.779	-112.089
350	416.958	649.002	592.020	19.944	452.465	675.196	-100.765
400	475.436	708.553	602.866	42.275	447.684	707.339	-92.367
450	528.521	767.671	617.900	67.397	443.534	740.050	-85.901
500	576.038	825.864	635.796	95.034	439.931	773.215	-80.776
600	655.806	938.227	676.920	156.784	434.065	840.453	-73.166
700	718.924	1044.245	721.901	225.641	429.774	908.551	-67.795
800	769.544	1143.668	768.476	300.153	426.875	977.150	-63.800
900	810.788	1236.768	815.392	379.238	425.187	1046.032	-60.709
1000	844.851	1324.011	861.939	462.072	424.545	1115.058	-58.243
1100	873.290	1405.907	907.707	548.021	424.750	1184.116	-56.228
1200	897.241	1482.950	952.466	636.581	425.658	1253.104	-54.545
1300	917.558	1555.591	996.093	727.348	427.085	1322.006	-53.118
1400	934.904	1624.241	1038.531	819.994	428.899	1390.787	-51.890
1500	949.798	1689.264	1079.765	914.247	431.016	1459.429	-50.821
1600	962.656	1750.983	1119.804	1009.886	433.307	1527.914	-49.880
1700	973.813	1809.686	1158.673	1106.722	435.695	1596.228	-49.045
1800	983.541	1865.629	1196.406	1204.601	438.106	1664.465	-48.301
1900	992.063	1919.040	1233.045	1303.390	440.507	1732.515	-47.629
2000	999.560	1970.121	1268.631	1402.979	442.844	1800.467	-47.022
2100	1006.184	2019.053	1303.209	1503.273	445.038	1868.290	-46.470
2200	1012.061	2065.999	1336.821	1604.191	447.088	1936.015	-45.966
2300	1017.294	2111.104	1369.511	1705.664	448.989	2003.650	-45.503
2400	1021.971	2154.501	1401.321	1807.631	450.668	2071.156	-45.077
2500	1026.165	2196.306	1432.289	1910.042	452.139	2138.714	-44.685
2600	1029.940	2236.628	1462.455	2012.850	453.364	2206.097	-44.320
2700	1033.347	2275.563	1491.853	2116.018	454.347	2273.512	-43.983
2800	1036.431	2313.200	1520.518	2219.509	455.062	2340.918	-43.669
2900	1039.232	2349.620	1548.484	2323.294	455.480	2408.248	-43.376
3000	1041.782	2384.895	1575.779	2427.347	455.644	2475.596	-43.103
3100	1044.109	2419.093	1602.434	2531.643	455.477	2542.864	-42.846
3200	1046.239	2452.276	1628.476	2636.162	455.019	2610.218	-42.607
3300	1048.192	2484.501	1653.930	2740.885	454.254	2677.632	-42.383
3400	1049.987	2515.820	1678.821	2845.795	453.153	2744.984	-42.171
3500	1051.640	2546.281	1703.173	2950.878	451.719	2812.355	-41.971
3600	1053.167	2575.928	1727.006	3056.119	449.976	2879.862	-41.785
3700	1054.578	2604.803	1750.342	3161.507	447.893	2947.438	-41.610
3800	1055.886	2632.944	1773.199	3267.032	445.441	3015.014	-41.443
3900	1057.101	2660.387	1795.597	3372.682	442.663	3082.606	-41.286
4000	1058.229	2687.165	1817.553	3478.449	439.542	3150.417	-41.139
4100	1059.281	2713.309	1839.083	3584.325	436.042	3218.233	-41.000
4200	1060.261	2738.847	1860.203	3690.303	432.192	3286.130	-40.868
4300	1061.177	2763.806	1880.928	3796.375	427.976	3354.031	-40.743
4400	1062.034	2788.212	1901.272	3902.536	423.405	3422.128	-40.625
4500	1062.837	2812.088	1921.248	4008.780	418.493	3490.391	-40.515
4600	1063.590	2835.456	1940.869	4115.102	413.187	3558.775	-40.410
4700	1064.297	2858.338	1960.147	4221.496	407.502	3627.162	-40.311
4800	1064.963	2880.752	1979.094	4327.960	401.485	3695.783	-40.217
4900	1065.589	2902.717	1997.720	4434.488	395.061	3764.393	-40.128
5000	1066.179	2924.251	2016.036	4541.076	388.325	3833.330	-40.046

3.362. Dibenzo[*de,qr*]pentacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-53-2
Point Group: C_s

Length: 16.75 Å
Width: 10.21 Å
Breadth: 3.889 Å
L/B Ratio: 1.641

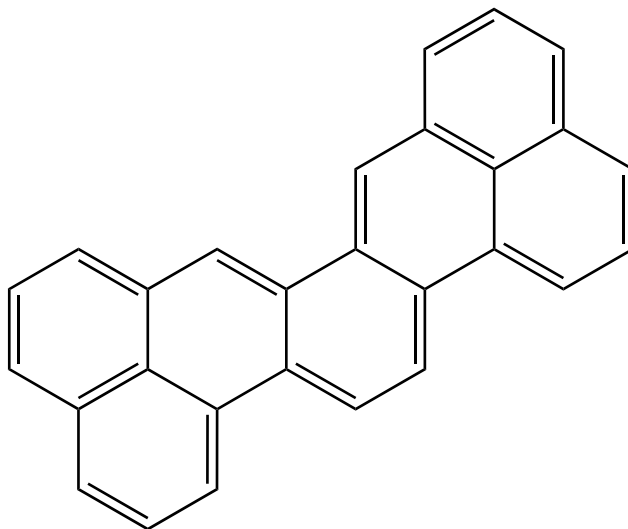
Cartesian coordinates:

C	-0.4904	-1.4077	0.0000	C	3.3037	-1.1907	0.0000	H	-5.5317	-1.6851	0.0000
C	0.8729	-0.8716	0.0000	C	3.5099	0.2189	0.0000	H	-4.7043	3.2320	0.0000
C	1.0410	0.5799	0.0000	C	2.4024	1.1181	0.0000	H	-2.3026	2.8454	0.0000
C	-0.0343	1.4037	0.0000	C	4.8257	0.7265	0.0000	H	0.1130	2.4967	0.0000
C	-1.3914	0.9031	0.0000	C	5.9194	-0.1773	0.0000	H	1.8066	-2.7887	0.0000
C	-1.5987	-0.5222	0.0000	C	5.6993	-1.5312	0.0000	H	4.2364	-3.1309	0.0000
C	-2.9081	-1.0362	0.0000	C	4.3883	-2.0457	0.0000	H	6.5437	-2.2285	0.0000
C	-4.0314	-0.1263	0.0000	C	5.0302	2.1324	0.0000	H	6.9390	0.2243	0.0000
C	-3.7977	1.2607	0.0000	C	3.9573	2.9829	0.0000	H	6.0554	2.5194	0.0000
C	-2.4565	1.7591	0.0000	C	2.6408	2.4774	0.0000	H	4.1078	4.0676	0.0000
C	-5.3625	-0.5974	0.0000	C	-0.7180	-2.7767	0.0000	H	1.7891	3.1750	0.0000
C	-6.4180	0.2844	0.0000	C	-2.0216	-3.2873	0.0000	H	-4.1317	-2.8205	0.0000
C	-6.1822	1.6702	0.0000	C	-3.1012	-2.4333	0.0000	H	-2.1749	-4.3714	0.0000
C	-4.8944	2.1527	0.0000	H	-7.0320	2.3606	0.0000	H	0.1410	-3.4653	0.0000
C	1.9492	-1.6954	0.0000	H	-7.4480	-0.0869	0.0000				

Table 3.362: Table of thermodynamic data as a function of temperature for Dibenzo[de,qr]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-52.452	493.414	493.414	∞
100	115.062	378.108	830.203	-45.210	519.696	565.133	-295.189
200	226.146	490.079	632.187	-28.422	505.804	616.107	-160.907
250	290.643	547.419	609.472	-15.513	499.256	644.440	-134.646
298.15	353.592	604.005	604.005	0.000	493.414	672.946	-117.895
300	355.983	606.200	604.012	0.656	493.198	674.059	-117.362
350	418.899	665.847	608.579	20.044	487.805	704.641	-105.160
400	477.320	725.654	619.477	42.471	483.120	735.936	-96.101
450	530.300	784.988	634.578	67.685	479.062	767.786	-89.120
500	577.696	843.362	652.547	95.407	475.545	800.080	-83.582
600	657.233	956.006	693.820	157.311	469.833	865.554	-75.352
700	720.164	1062.229	738.942	226.301	465.675	931.863	-69.535
800	770.640	1161.808	785.645	300.930	462.892	998.655	-65.204
900	811.769	1255.030	832.677	380.118	461.308	1065.717	-61.851
1000	845.738	1342.372	879.326	463.046	460.760	1132.912	-59.176
1100	874.097	1424.349	925.186	549.080	461.049	1200.129	-56.988
1200	897.978	1501.459	970.028	637.717	462.034	1267.270	-55.162
1300	918.234	1574.157	1013.730	728.555	463.532	1334.318	-53.612
1400	935.524	1642.855	1056.237	821.265	465.411	1401.240	-52.280
1500	950.368	1707.918	1097.533	915.578	467.588	1468.019	-51.120
1600	963.181	1769.672	1137.628	1011.271	469.932	1534.636	-50.100
1700	974.297	1828.406	1176.549	1108.158	472.371	1601.079	-49.194
1800	983.989	1884.376	1214.330	1206.083	474.828	1667.444	-48.387
1900	992.477	1937.810	1251.012	1304.915	477.273	1733.618	-47.659
2000	999.944	1988.911	1286.639	1404.544	479.650	1799.691	-47.002
2100	1006.541	2037.862	1321.254	1504.875	481.881	1865.635	-46.404
2200	1012.393	2084.824	1354.902	1605.827	483.965	1931.478	-45.858
2300	1017.603	2129.943	1387.625	1707.332	485.898	1997.229	-45.358
2400	1022.260	2173.352	1419.465	1809.330	487.607	2062.851	-44.896
2500	1026.435	2215.169	1450.462	1911.768	489.106	2128.523	-44.472
2600	1030.193	2255.501	1480.654	2014.603	490.356	2194.019	-44.077
2700	1033.584	2294.446	1510.077	2117.794	491.364	2259.546	-43.713
2800	1036.655	2332.091	1538.767	2221.309	492.103	2325.063	-43.374
2900	1039.442	2368.518	1566.754	2325.116	492.542	2390.504	-43.057
3000	1041.980	2403.800	1594.071	2429.189	492.727	2455.962	-42.761
3100	1044.296	2438.005	1620.745	2533.505	492.578	2521.339	-42.483
3200	1046.416	2471.194	1646.806	2638.042	492.140	2586.802	-42.224
3300	1048.359	2503.424	1672.278	2742.782	491.392	2652.324	-41.982
3400	1050.146	2534.748	1697.186	2847.708	490.306	2717.783	-41.753
3500	1051.791	2565.213	1721.554	2952.806	488.888	2783.261	-41.537
3600	1053.310	2594.864	1745.403	3058.062	487.160	2848.874	-41.335
3700	1054.715	2623.743	1768.753	3163.465	485.090	2914.557	-41.145
3800	1056.016	2651.888	1791.625	3269.002	482.652	2980.239	-40.965
3900	1057.224	2679.335	1814.036	3374.665	479.886	3045.936	-40.795
4000	1058.347	2706.115	1836.005	3480.444	476.778	3111.852	-40.636
4100	1059.393	2732.262	1857.547	3586.332	473.289	3177.773	-40.484
4200	1060.369	2757.803	1878.679	3692.320	469.450	3243.775	-40.341
4300	1061.280	2782.764	1899.415	3798.403	465.245	3309.780	-40.205
4400	1062.133	2807.173	1919.769	3904.574	460.684	3375.981	-40.077
4500	1062.932	2831.051	1939.756	4010.828	455.782	3442.348	-39.957
4600	1063.681	2854.421	1959.386	4117.159	450.485	3508.836	-39.843
4700	1064.385	2877.304	1978.674	4223.563	444.809	3575.326	-39.734
4800	1065.047	2899.720	1997.630	4330.035	438.800	3642.050	-39.633
4900	1065.670	2921.687	2016.265	4436.571	432.385	3708.763	-39.535
5000	1066.257	2943.223	2034.589	4543.167	425.657	3775.803	-39.445

3.363. Dibenzo[*de,kl*]pentaphene



Formula: $C_{28}H_{16}$
Mass: 352.427 g/mol
CAS Number: 83786-06-5
Point Group: C_{2v}

Length: 15.99 Å
Width: 9.174 Å
Breadth: 3.884 Å
L/B Ratio: 1.743

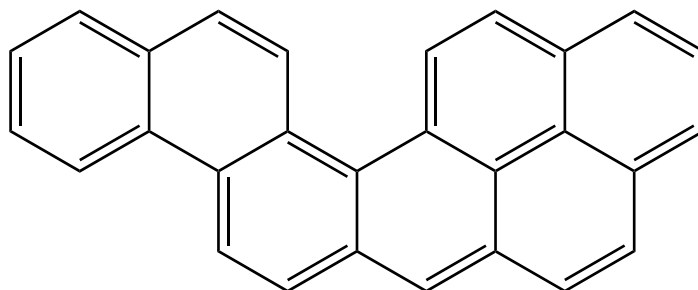
Cartesian coordinates:

C	-5.6988	1.0666	0.0000	C	1.4244	1.0708	0.0000	H	3.0320	-3.5516	0.0000
C	-4.9965	-0.1681	0.0000	C	0.7319	-0.2114	0.0000	H	0.8966	-2.3401	0.0000
C	-3.5861	-0.1610	0.0000	C	2.8855	1.0736	0.0000	H	1.2478	3.1978	0.0000
C	-2.8832	1.0800	0.0000	C	3.5858	-0.1688	0.0000	H	-1.2407	3.2005	0.0000
C	-3.6001	2.2599	0.0000	C	2.8756	-1.4040	0.0000	H	6.7968	1.0389	0.0000
C	-5.0096	2.2503	0.0000	C	1.4317	-1.3762	0.0000	H	5.5527	3.1930	0.0000
C	-2.8787	-1.3977	0.0000	C	4.9962	-0.1790	0.0000	H	3.0657	3.2120	0.0000
C	-3.5771	-2.5899	0.0000	C	5.6816	-1.4213	0.0000	H	-0.9017	-2.3381	0.0000
C	-4.9853	-2.5890	0.0000	C	4.9796	-2.5999	0.0000	H	-6.7805	-1.4074	0.0000
C	-5.6847	-1.4089	0.0000	C	3.5714	-2.5978	0.0000	H	-5.5171	-3.5463	0.0000
C	-1.4220	1.0739	0.0000	C	3.6049	2.2521	0.0000	H	-3.0397	-3.5449	0.0000
C	-0.7324	-0.2098	0.0000	C	5.0145	2.2394	0.0000	H	-3.0588	3.2187	0.0000
C	-1.4347	-1.3731	0.0000	C	5.7012	1.0542	0.0000	H	-5.5458	3.2051	0.0000
C	-0.7116	2.2348	0.0000	H	5.5094	-3.5584	0.0000	H	-6.7945	1.0537	0.0000
C	0.7165	2.2332	0.0000	H	6.7774	-1.4222	0.0000				

Table 3.363: Table of thermodynamic data as a function of temperature for Dibenzo[de,kl]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-52.221	546.059	546.059	∞
100	113.924	356.501	807.882	-45.138	572.413	620.010	-323.853
200	225.854	467.920	610.043	-28.425	558.446	673.181	-175.813
250	290.698	525.234	587.322	-15.522	551.893	702.623	-146.802
298.15	353.880	581.851	581.851	0.000	546.059	732.197	-128.275
300	356.278	584.047	581.858	0.657	545.844	733.350	-127.685
350	419.359	643.753	586.429	20.063	540.470	765.038	-114.173
400	477.891	703.630	597.339	42.516	535.811	797.436	-104.132
450	530.938	763.035	612.456	67.761	531.784	830.386	-96.387
500	578.369	821.478	630.446	95.516	528.299	863.776	-90.236
600	657.912	934.247	671.766	157.489	522.656	931.431	-81.087
700	720.804	1040.572	716.937	226.544	518.563	999.911	-74.613
800	771.223	1140.233	763.689	301.235	515.842	1068.865	-69.788
900	812.293	1233.520	810.767	380.478	514.313	1138.081	-66.051
1000	846.206	1320.914	857.459	463.456	513.815	1207.424	-63.068
1100	874.514	1402.934	903.358	549.533	514.148	1276.785	-60.628
1200	898.350	1480.077	948.236	638.210	515.173	1346.066	-58.592
1300	918.567	1552.804	991.971	729.083	516.706	1415.250	-56.864
1400	935.822	1621.525	1034.507	821.824	518.615	1484.306	-55.379
1500	950.637	1686.608	1075.831	916.166	520.821	1553.217	-54.087
1600	963.424	1748.379	1115.951	1011.884	523.191	1621.965	-52.951
1700	974.518	1807.127	1154.895	1108.794	525.653	1690.537	-51.943
1800	984.189	1863.108	1192.697	1206.741	528.132	1759.028	-51.045
1900	992.660	1916.553	1229.399	1305.592	530.595	1827.329	-50.236
2000	1000.112	1967.663	1265.044	1405.239	532.990	1895.528	-49.505
2100	1006.695	2016.621	1299.676	1505.586	535.237	1963.595	-48.841
2200	1012.535	2063.590	1333.339	1606.553	537.336	2031.562	-48.234
2300	1017.735	2108.716	1366.076	1708.071	539.282	2099.437	-47.679
2400	1022.381	2152.130	1397.930	1810.081	541.004	2167.181	-47.166
2500	1026.549	2193.952	1428.939	1912.532	542.515	2234.974	-46.696
2600	1030.298	2234.288	1459.143	2015.377	543.776	2302.592	-46.259
2700	1033.683	2273.237	1488.578	2118.579	544.794	2370.241	-45.854
2800	1036.747	2310.886	1517.277	2222.103	545.542	2437.878	-45.478
2900	1039.529	2347.316	1545.275	2325.919	545.990	2505.440	-45.127
3000	1042.061	2382.601	1572.600	2430.001	546.184	2573.018	-44.799
3100	1044.372	2416.808	1599.284	2534.324	546.043	2640.515	-44.491
3200	1046.487	2449.999	1625.353	2638.868	545.611	2708.097	-44.204
3300	1048.427	2482.232	1650.833	2743.616	544.871	2775.738	-43.935
3400	1050.210	2513.557	1675.749	2848.549	543.792	2843.317	-43.681
3500	1051.852	2544.024	1700.123	2953.653	542.380	2910.914	-43.442
3600	1053.368	2573.677	1723.979	3058.915	540.658	2978.646	-43.218
3700	1054.769	2602.558	1747.335	3164.322	538.594	3046.447	-43.007
3800	1056.068	2630.704	1770.213	3269.865	536.160	3114.247	-42.807
3900	1057.274	2658.152	1792.630	3375.533	533.400	3182.063	-42.618
4000	1058.394	2684.934	1814.605	3481.317	530.296	3250.097	-42.441
4100	1059.438	2711.081	1836.152	3587.209	526.812	3318.136	-42.273
4200	1060.412	2736.623	1857.289	3693.202	522.977	3386.256	-42.113
4300	1061.321	2761.586	1878.030	3799.290	518.777	3454.379	-41.962
4400	1062.172	2785.995	1898.389	3905.465	514.220	3522.698	-41.819
4500	1062.969	2809.874	1918.380	4011.722	509.321	3591.182	-41.684
4600	1063.717	2833.245	1938.015	4118.057	504.028	3659.788	-41.557
4700	1064.419	2856.129	1957.307	4224.464	498.355	3728.396	-41.436
4800	1065.080	2878.546	1976.267	4330.939	492.350	3797.237	-41.322
4900	1065.701	2900.514	1994.906	4437.479	485.938	3866.068	-41.212
5000	1066.287	2922.050	2013.234	4544.078	479.213	3935.226	-41.110

3.364. Benzo[*mno*]naphtho[1,2-*c*]chrysene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-49-6
Point Group: C₁

Length: 16.78 Å
Width: 9.464 Å
Breadth: 4.920 Å
L/B Ratio: 1.773

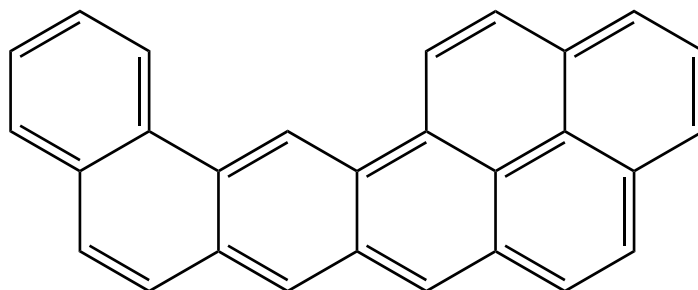
Cartesian coordinates:

C	5.8291	1.7712	0.0464	C	-0.1661	-1.8923	0.0610	H	4.6181	3.5133	0.4299
C	5.8521	0.3908	-0.1591	C	-1.3398	-2.6944	0.2188	H	5.6382	-2.2665	-0.5056
C	4.6322	2.4311	0.2588	C	-2.5638	-2.1171	0.2942	H	3.5226	-3.5649	-0.4560
C	4.6677	-0.3401	-0.1622	C	-1.5817	0.0910	-0.1021	H	1.1070	-3.6450	-0.0772
C	4.6722	-1.7722	-0.3513	C	-2.7131	-0.7107	0.0964	H	0.0629	2.1795	0.6732
C	3.5227	-2.4763	-0.3274	C	-3.0339	1.9860	-0.6161	H	2.1699	3.4269	0.7520
C	2.2473	-1.8227	-0.1354	C	-1.7919	1.4440	-0.5208	H	-1.2255	-3.7819	0.2979
C	1.0798	-2.5482	-0.0498	C	-4.1914	1.2160	-0.2932	H	-3.4685	-2.7191	0.4688
C	3.4308	0.3252	0.0320	C	-4.0355	-0.1382	0.0501	H	-3.1695	3.0214	-0.9495
C	2.1960	-0.4050	0.0053	C	-5.1932	-0.9014	0.3406	H	-0.9213	2.0548	-0.7962
C	0.9622	0.2596	0.1374	C	-6.4398	-0.3285	0.3001	H	-5.0713	-1.9639	0.5997
C	1.0059	1.6618	0.4501	C	-6.5880	1.0309	-0.0378	H	-7.3295	-0.9240	0.5297
C	2.1674	2.3589	0.5048	C	-5.4839	1.7913	-0.3322	H	-7.5899	1.4717	-0.0640
C	3.4233	1.7165	0.2574	H	6.7695	2.3324	0.0434	H	-5.5873	2.8492	-0.5989
C	-0.2589	-0.4837	0.0312	H	6.8086	-0.1206	-0.3164				

Table 3.364: Table of thermodynamic data as a function of temperature for Benzo[*mno*]naphtho[1,2-*c*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.401	463.004	463.004	∞
100	110.316	353.033	799.273	-44.624	489.872	537.816	-280.920
200	223.360	462.246	603.357	-28.222	475.594	591.463	-154.471
250	288.672	519.058	580.784	-15.432	468.928	621.202	-129.790
298.15	352.123	575.343	575.343	0.000	463.004	651.082	-114.064
300	354.530	577.529	575.350	0.654	462.785	652.247	-113.564
350	417.775	636.978	579.901	19.977	457.329	684.268	-102.119
400	476.414	696.651	590.766	42.354	452.593	717.010	-93.630
450	529.546	755.887	605.829	67.526	448.494	750.313	-87.092
500	577.053	814.188	623.759	95.214	444.942	784.064	-81.909
600	656.741	926.729	664.959	157.062	439.174	852.461	-74.212
700	719.770	1032.884	710.016	226.008	434.971	921.701	-68.777
800	770.314	1132.415	756.663	300.601	432.153	991.431	-64.732
900	811.492	1225.602	803.647	379.759	430.539	1061.434	-61.603
1000	845.499	1312.917	850.255	462.661	429.965	1131.572	-59.106
1100	873.888	1394.873	896.079	548.672	430.232	1201.736	-57.065
1200	897.793	1471.965	940.890	637.290	431.198	1271.826	-55.360
1300	918.069	1544.649	984.564	728.110	432.678	1341.824	-53.914
1400	935.376	1613.335	1027.046	820.805	434.541	1411.697	-52.670
1500	950.234	1678.389	1068.320	915.104	436.704	1481.428	-51.587
1600	963.060	1740.135	1108.395	1010.784	439.036	1550.999	-50.634
1700	974.187	1798.862	1147.298	1107.659	441.463	1620.396	-49.788
1800	983.888	1854.826	1185.062	1205.574	443.910	1689.715	-49.033
1900	992.385	1908.254	1221.730	1304.397	446.345	1758.845	-48.353
2000	999.859	1959.351	1257.343	1404.017	448.713	1827.874	-47.738
2100	1006.463	2008.298	1291.945	1504.340	450.936	1896.774	-47.179
2200	1012.320	2055.256	1325.581	1605.285	453.012	1965.574	-46.668
2300	1017.536	2100.373	1358.293	1706.783	454.938	2034.282	-46.199
2400	1022.197	2143.779	1390.123	1808.774	456.641	2102.861	-45.767
2500	1026.378	2185.593	1421.111	1911.206	458.134	2171.490	-45.370
2600	1030.139	2225.923	1451.294	2014.035	459.379	2239.944	-45.000
2700	1033.534	2264.866	1480.710	2117.222	460.381	2308.429	-44.658
2800	1036.607	2302.509	1509.391	2220.731	461.115	2376.904	-44.341
2900	1039.398	2338.935	1537.372	2324.534	461.549	2445.304	-44.044
3000	1041.938	2374.216	1564.681	2428.602	461.730	2513.720	-43.767
3100	1044.257	2408.419	1591.350	2532.914	461.578	2582.056	-43.506
3200	1046.378	2441.607	1617.404	2637.447	461.135	2650.477	-43.264
3300	1048.324	2473.836	1642.871	2742.184	460.383	2718.957	-43.037
3400	1050.112	2505.158	1667.774	2847.107	459.295	2787.376	-42.822
3500	1051.760	2535.622	1692.136	2952.202	457.873	2855.813	-42.620
3600	1053.280	2565.273	1715.980	3057.455	456.142	2924.385	-42.431
3700	1054.686	2594.151	1739.326	3162.854	454.070	2993.027	-42.253
3800	1055.989	2622.295	1762.193	3268.388	451.628	3061.668	-42.085
3900	1057.199	2649.741	1784.600	3374.049	448.860	3130.324	-41.925
4000	1058.323	2676.521	1806.565	3479.825	445.749	3199.199	-41.776
4100	1059.370	2702.667	1828.104	3585.711	442.258	3268.080	-41.635
4200	1060.347	2728.207	1849.232	3691.697	438.417	3337.041	-41.501
4300	1061.259	2753.169	1869.964	3797.778	434.210	3406.006	-41.374
4400	1062.113	2777.576	1890.316	3903.947	429.647	3475.167	-41.255
4500	1062.912	2801.454	1910.299	4010.199	424.742	3544.493	-41.143
4600	1063.662	2824.824	1929.927	4116.528	419.443	3613.941	-41.037
4700	1064.367	2847.707	1949.211	4222.930	413.765	3683.391	-40.935
4800	1065.029	2870.123	1968.164	4329.400	407.755	3753.074	-40.841
4900	1065.653	2892.089	1986.796	4435.934	401.338	3822.747	-40.750
5000	1066.241	2913.624	2005.118	4542.529	394.609	3892.748	-40.666

3.365. Benzo[*a*]naphtho[8,1,2-*lmn*]naphthacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 190-01-2
Point Group: C_s

Length: 16.64 Å
Width: 9.548 Å
Breadth: 3.888 Å
L/B Ratio: 1.743

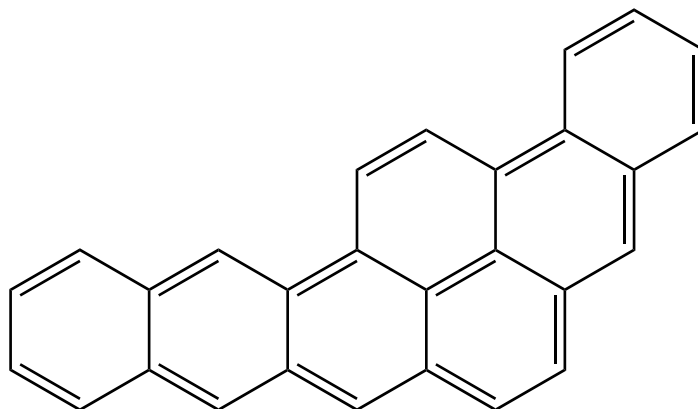
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C	-6.2563	1.9143	0.0000	C	2.2670	-1.7580	0.0000	H	-2.8881	2.4840	0.0000
C	-6.2523	0.5343	0.0000	C	3.5158	-2.4933	0.0000	H	-5.0599	3.7167	0.0000
C	-3.8467	1.9424	0.0000	C	4.7051	-1.8603	0.0000	H	-5.9904	-2.1346	0.0000
C	-5.0471	2.6219	0.0000	C	4.7870	-0.4150	0.0000	H	-3.8559	-3.3983	0.0000
C	-3.8210	0.5352	0.0000	C	6.0090	0.2432	0.0000	H	-1.4216	-3.4278	0.0000
C	-5.0351	-0.1723	0.0000	C	6.0574	1.6424	0.0000	H	-1.3197	1.5684	0.0000
C	-5.0254	-1.6147	0.0000	C	4.8964	2.3882	0.0000	H	1.0094	-3.4988	0.0000
C	-3.8639	-2.3021	0.0000	C	3.5846	0.3390	0.0000	H	3.4592	-3.5881	0.0000
C	-2.5657	-0.1957	0.0000	C	3.6419	1.7477	0.0000	H	5.6458	-2.4230	0.0000
C	-2.5928	-1.6177	0.0000	C	2.4193	2.4924	0.0000	H	6.9415	-0.3324	0.0000
C	-1.4021	-2.3307	0.0000	C	1.2193	1.8546	0.0000	H	7.0306	2.1447	0.0000
C	-1.3437	0.4616	0.0000	C	1.1376	0.4260	0.0000	H	4.9394	3.4832	0.0000
C	-0.1321	-0.2483	0.0000	C	2.3155	-0.3228	0.0000	H	2.4748	3.5869	0.0000
C	-0.1630	-1.6646	0.0000	H	-7.2040	2.4625	0.0000	H	0.2731	2.4177	0.0000
C	1.0571	-2.4027	0.0000	H	-7.1963	-0.0224	0.0000				

Table 3.365: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[8,1,2-*lmn*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.576	442.535	442.535	∞
100	111.441	355.817	802.836	-44.702	469.325	516.990	-270.042
200	223.694	465.549	606.698	-28.230	455.117	570.325	-148.951
250	288.738	522.406	584.123	-15.429	448.461	599.898	-125.339
298.15	351.973	578.684	578.684	0.000	442.535	629.617	-110.304
300	354.372	580.869	578.691	0.653	442.316	630.776	-109.826
350	417.430	640.279	583.239	19.964	436.847	662.631	-98.890
400	475.928	699.896	594.096	42.320	432.090	695.209	-90.783
450	528.965	759.069	609.146	67.466	427.964	728.351	-84.543
500	576.420	817.306	627.060	95.123	424.382	761.945	-79.598
600	656.098	929.729	668.219	156.906	418.549	830.035	-72.260
700	719.183	1035.789	713.232	225.790	414.285	898.981	-67.081
800	769.809	1135.247	759.835	300.329	411.411	968.424	-63.230
900	811.070	1228.379	806.778	379.441	409.751	1038.146	-60.251
1000	845.152	1315.653	853.349	462.304	409.139	1108.010	-57.875
1100	873.605	1397.579	899.139	548.284	409.374	1177.902	-55.933
1200	897.562	1474.649	943.919	636.876	410.314	1247.721	-54.311
1300	917.880	1547.316	987.566	727.675	411.774	1317.452	-52.935
1400	935.220	1615.990	1030.024	820.353	413.619	1387.059	-51.751
1500	950.106	1681.034	1071.275	914.637	415.768	1456.526	-50.720
1600	962.954	1742.772	1111.331	1010.306	418.089	1525.832	-49.812
1700	974.098	1801.493	1150.216	1107.172	420.506	1594.966	-49.006
1800	983.813	1857.452	1187.965	1205.078	422.945	1664.022	-48.288
1900	992.321	1910.877	1224.617	1303.894	425.373	1732.889	-47.639
2000	999.806	1961.971	1260.217	1403.508	427.735	1801.657	-47.053
2100	1006.417	2010.915	1294.807	1503.826	429.953	1870.294	-46.520
2200	1012.281	2057.872	1328.432	1604.767	432.025	1938.833	-46.033
2300	1017.502	2102.987	1361.134	1706.261	433.947	2007.279	-45.586
2400	1022.168	2146.391	1392.955	1808.249	435.647	2075.597	-45.173
2500	1026.352	2188.205	1423.933	1910.678	437.137	2143.965	-44.795
2600	1030.116	2228.534	1454.109	2013.505	438.379	2212.158	-44.442
2700	1033.514	2267.475	1483.516	2116.689	439.380	2280.382	-44.116
2800	1036.589	2305.118	1512.191	2220.197	440.111	2348.596	-43.813
2900	1039.382	2341.543	1540.165	2323.998	440.544	2416.735	-43.529
3000	1041.924	2376.823	1567.468	2428.065	440.724	2484.890	-43.265
3100	1044.244	2411.026	1594.131	2532.375	440.570	2552.965	-43.016
3200	1046.367	2444.214	1620.180	2636.907	440.126	2621.126	-42.785
3300	1048.314	2476.442	1645.641	2741.643	439.373	2689.346	-42.568
3400	1050.103	2507.764	1670.540	2846.565	438.283	2757.503	-42.363
3500	1051.751	2538.228	1694.897	2951.658	436.861	2825.680	-42.170
3600	1053.272	2567.879	1718.737	3056.911	435.129	2893.991	-41.990
3700	1054.679	2596.757	1742.079	3162.309	433.056	2962.373	-41.820
3800	1055.983	2624.901	1764.942	3267.843	430.614	3030.753	-41.660
3900	1057.193	2652.346	1787.346	3373.503	427.845	3099.149	-41.508
4000	1058.317	2679.126	1809.307	3479.279	424.733	3167.764	-41.366
4100	1059.365	2705.272	1830.842	3585.163	421.242	3236.384	-41.231
4200	1060.342	2730.812	1851.967	3691.149	417.400	3305.085	-41.104
4300	1061.255	2755.773	1872.697	3797.230	413.192	3373.789	-40.983
4400	1062.109	2780.181	1893.045	3903.398	408.629	3442.689	-40.869
4500	1062.908	2804.058	1913.025	4009.650	403.724	3511.755	-40.763
4600	1063.659	2827.428	1932.650	4115.978	398.425	3580.943	-40.662
4700	1064.363	2850.311	1951.933	4222.380	392.746	3650.132	-40.566
4800	1065.026	2872.727	1970.883	4328.850	386.736	3719.555	-40.476
4900	1065.650	2894.693	1989.513	4435.384	380.318	3788.968	-40.390
5000	1066.238	2916.228	2007.833	4541.978	373.589	3858.708	-40.311

3.366. Benzo[*vwx*]hexaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 2828-72-0
Point Group: C_s

Length: 18.08 Å
Width: 9.869 Å
Breadth: 3.884 Å
L/B Ratio: 1.832

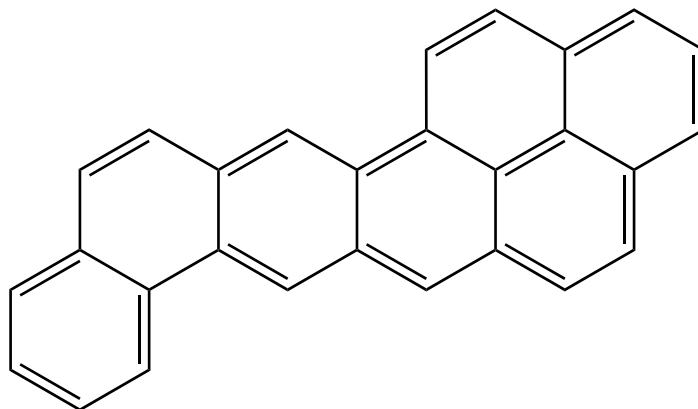
Cartesian coordinates:

C	6.4450	-1.8597	0.0000	C	-4.0457	1.4884	0.0000	H	6.4727	1.5618	0.0000
C	6.9476	-0.5285	0.0000	C	-3.7529	-0.9493	0.0000	H	4.7070	-3.1145	0.0000
C	6.0948	0.5332	0.0000	C	-4.6015	0.1739	0.0000	H	4.1718	2.4281	0.0000
C	5.1032	-2.0928	0.0000	C	-6.0054	-0.0138	0.0000	H	2.3977	-2.2461	0.0000
C	4.1788	-1.0015	0.0000	C	-6.5368	-1.2796	0.0000	H	1.9054	3.3031	0.0000
C	4.6794	0.3253	0.0000	C	-5.6892	-2.4046	0.0000	H	-0.3595	4.2105	0.0000
C	3.7829	1.4022	0.0000	C	-4.3259	-2.2431	0.0000	H	-2.8088	3.8578	0.0000
C	2.7944	-1.2180	0.0000	C	0.4700	-0.3564	0.0000	H	-4.7285	2.3472	0.0000
C	1.9027	-0.1494	0.0000	C	-0.3919	0.7433	0.0000	H	-6.6595	0.8657	0.0000
C	2.4072	1.1815	0.0000	C	-1.8030	0.5439	0.0000	H	-7.6219	-1.4257	0.0000
C	1.4923	2.2865	0.0000	C	-2.3261	-0.7563	0.0000	H	-6.1279	-3.4077	0.0000
C	0.1435	2.0837	0.0000	C	-1.4319	-1.8595	0.0000	H	-3.6495	-3.1117	0.0000
C	-0.7848	3.2000	0.0000	C	-0.0795	-1.6656	0.0000	H	-1.8613	-2.8733	0.0000
C	-2.1154	3.0085	0.0000	H	7.1574	-2.6912	0.0000	H	0.6159	-2.5192	0.0000
C	-2.6899	1.6756	0.0000	H	8.0318	-0.3753	0.0000				

Table 3.366: Table of thermodynamic data as a function of temperature for Benzo[*vw*x]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-52.157	453.748	453.748	∞
100	113.559	361.492	812.266	-45.077	480.163	527.261	-275.407
200	225.570	472.663	614.659	-28.399	466.161	579.947	-151.463
250	290.451	529.920	591.957	-15.509	459.595	609.153	-127.273
298.15	353.592	586.491	586.491	0.000	453.748	638.503	-111.861
300	355.987	588.685	586.497	0.656	453.533	639.648	-111.370
350	418.970	648.339	591.065	20.046	448.142	671.105	-100.155
400	477.391	708.156	601.965	42.477	443.461	703.275	-91.836
450	530.346	767.498	617.067	67.694	439.406	736.000	-85.431
500	577.712	825.875	635.039	95.418	435.890	769.169	-80.353
600	657.213	938.518	676.316	157.321	430.178	836.391	-72.813
700	720.138	1044.737	721.440	226.308	426.017	904.449	-67.489
800	770.626	1144.313	768.144	300.936	423.232	972.991	-63.528
900	811.774	1237.535	815.176	380.123	421.648	1041.802	-60.463
1000	845.761	1324.878	861.826	463.053	421.101	1110.747	-58.018
1100	874.135	1406.858	907.687	549.089	421.393	1179.713	-56.019
1200	898.028	1483.972	952.529	637.730	422.383	1248.603	-54.349
1300	918.291	1556.674	996.233	728.574	423.886	1317.399	-52.933
1400	935.586	1625.376	1038.741	821.290	425.770	1386.069	-51.714
1500	950.433	1690.444	1080.038	915.609	427.954	1454.596	-50.652
1600	963.247	1752.203	1120.135	1011.309	430.305	1522.960	-49.719
1700	974.363	1810.941	1159.057	1108.202	432.751	1591.150	-48.889
1800	984.054	1866.914	1196.840	1206.134	435.214	1659.261	-48.150
1900	992.540	1920.352	1233.524	1304.973	437.665	1727.181	-47.483
2000	1000.005	1971.456	1269.152	1404.608	440.048	1795.000	-46.880
2100	1006.600	2020.409	1303.769	1504.945	442.285	1862.689	-46.331
2200	1012.449	2067.374	1337.418	1605.903	444.376	1930.278	-45.830
2300	1017.657	2112.496	1370.143	1707.413	446.314	1997.774	-45.370
2400	1022.311	2155.907	1401.984	1809.416	448.029	2065.140	-44.946
2500	1026.485	2197.726	1432.983	1911.860	449.532	2132.556	-44.556
2600	1030.240	2238.060	1463.176	2014.699	450.788	2199.796	-44.194
2700	1033.629	2277.007	1492.601	2117.896	451.800	2267.068	-43.858
2800	1036.698	2314.654	1521.291	2221.414	452.543	2334.329	-43.547
2900	1039.483	2351.082	1549.280	2325.226	452.986	2401.513	-43.255
3000	1042.019	2386.366	1576.598	2429.303	453.175	2468.715	-42.983
3100	1044.333	2420.571	1603.274	2533.622	453.030	2535.835	-42.728
3200	1046.451	2453.762	1629.336	2638.163	452.595	2603.041	-42.489
3300	1048.393	2485.993	1654.809	2742.906	451.851	2670.306	-42.267
3400	1050.178	2517.317	1679.718	2847.836	450.769	2737.509	-42.056
3500	1051.822	2547.783	1704.087	2952.937	449.354	2804.730	-41.857
3600	1053.340	2577.436	1727.937	3058.196	447.629	2872.086	-41.672
3700	1054.743	2606.316	1751.288	3163.601	445.562	2939.512	-41.498
3800	1056.043	2634.461	1774.161	3269.141	443.126	3006.936	-41.332
3900	1057.250	2661.908	1796.573	3374.807	440.363	3074.376	-41.176
4000	1058.372	2688.690	1818.543	3480.589	437.257	3142.034	-41.030
4100	1059.417	2714.837	1840.086	3586.479	433.771	3209.698	-40.891
4200	1060.392	2740.378	1861.218	3692.470	429.934	3277.442	-40.760
4300	1061.302	2765.340	1881.955	3798.555	425.731	3345.190	-40.635
4400	1062.154	2789.749	1902.311	3904.728	421.173	3413.133	-40.518
4500	1062.952	2813.628	1922.298	4010.984	416.272	3481.242	-40.408
4600	1063.700	2836.998	1941.929	4117.317	410.977	3549.473	-40.305
4700	1064.403	2859.882	1961.218	4223.723	405.303	3617.705	-40.205
4800	1065.065	2882.298	1980.174	4330.196	399.297	3686.171	-40.113
4900	1065.687	2904.266	1998.810	4436.734	392.883	3754.626	-40.024
5000	1066.274	2925.802	2017.135	4543.333	386.157	3823.409	-39.942

3.367. Benzo[*a*]naphtho[2,1,8-*hij*]naphthacene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 190-05-6
Point Group: C_s

Length: 17.98 Å
Width: 9.542 Å
Breadth: 3.884 Å
L/B Ratio: 1.884

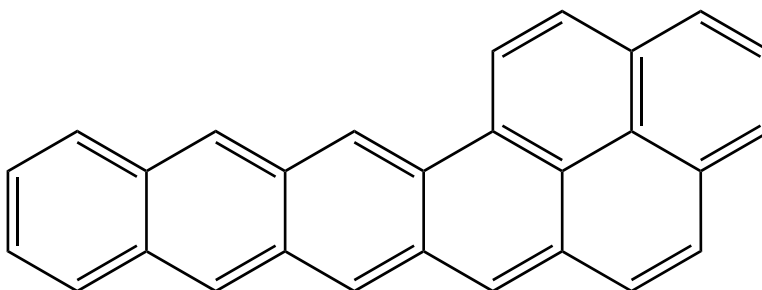
Cartesian coordinates:

C	6.4424	-0.4488	0.0000	C	-1.8911	1.6263	0.0000	H	6.3705	2.9487	0.0000
C	6.9030	0.8520	0.0000	C	-2.8714	2.6936	0.0000	H	3.9137	2.5046	0.0000
C	5.9962	1.9199	0.0000	C	-4.1936	2.4346	0.0000	H	2.8801	-3.3669	0.0000
C	4.6384	1.6760	0.0000	C	-4.6929	1.0759	0.0000	H	5.3126	-2.8805	0.0000
C	5.0599	-0.7126	0.0000	C	-6.0536	0.8023	0.0000	H	2.1353	2.1510	0.0000
C	4.1482	0.3568	0.0000	C	-6.5077	-0.5220	0.0000	H	0.5635	-2.5926	0.0000
C	3.2503	-2.3351	0.0000	C	-5.6144	-1.5737	0.0000	H	-0.1808	2.9251	0.0000
C	4.5739	-2.0706	0.0000	C	-3.7623	0.0043	0.0000	H	-2.4983	3.7244	0.0000
C	2.2776	-1.2689	0.0000	C	-4.2278	-1.3265	0.0000	H	-4.9295	3.2470	0.0000
C	2.7213	0.0825	0.0000	C	-3.2752	-2.3951	0.0000	H	-6.7779	1.6247	0.0000
C	1.7844	1.1061	0.0000	C	-1.9415	-2.1347	0.0000	H	-7.5850	-0.7189	0.0000
C	0.9183	-1.5491	0.0000	C	-1.4467	-0.7921	0.0000	H	-5.9747	-2.6087	0.0000
C	-0.0353	-0.5173	0.0000	C	-2.3553	0.2674	0.0000	H	-3.6472	-3.4259	0.0000
C	0.4059	0.8289	0.0000	H	7.1489	-1.2867	0.0000	H	-1.2010	-2.9496	0.0000
C	-0.5459	1.8905	0.0000	H	7.9788	1.0556	0.0000				

Table 3.367: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[2,1,8-*hij*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-52.075	441.038	441.038	∞
100	112.938	362.329	812.441	-45.011	467.519	514.534	-268.759
200	225.221	473.073	615.037	-28.393	453.458	567.161	-148.124
250	290.404	530.284	592.335	-15.513	446.882	596.349	-124.598
298.15	353.767	586.867	586.867	0.000	441.038	625.681	-109.614
300	356.170	589.063	586.874	0.657	440.823	626.825	-109.138
350	419.315	648.758	591.444	20.060	435.446	658.263	-98.238
400	477.843	708.629	602.352	42.511	430.785	690.410	-90.156
450	530.861	768.027	617.467	67.752	426.754	723.110	-83.935
500	578.260	826.460	635.455	95.503	423.265	756.251	-79.003
600	657.764	939.205	676.768	157.462	417.608	823.409	-71.683
700	720.655	1045.507	721.932	226.502	413.501	891.394	-66.515
800	771.096	1145.149	768.675	301.179	410.766	959.856	-62.671
900	812.195	1238.423	815.744	380.411	409.226	1028.581	-59.696
1000	846.137	1325.808	862.428	463.380	408.719	1097.434	-57.323
1100	874.471	1407.822	908.320	549.452	409.047	1166.306	-55.382
1200	898.328	1484.963	953.192	638.125	410.068	1235.098	-53.761
1300	918.561	1557.688	996.921	728.997	411.600	1303.794	-52.386
1400	935.829	1626.410	1039.453	821.739	413.509	1372.361	-51.202
1500	950.652	1691.493	1080.772	916.081	415.716	1440.784	-50.172
1600	963.446	1753.265	1120.889	1011.802	418.088	1509.043	-49.264
1700	974.544	1812.015	1159.830	1108.714	420.553	1577.126	-48.458
1800	984.218	1867.998	1197.630	1206.663	423.034	1645.129	-47.739
1900	992.691	1921.444	1234.330	1305.518	425.500	1712.940	-47.091
2000	1000.143	1972.556	1269.972	1405.167	427.898	1780.650	-46.505
2100	1006.727	2021.516	1304.603	1505.517	430.148	1848.228	-45.971
2200	1012.567	2068.486	1338.264	1606.488	432.250	1915.706	-45.484
2300	1017.766	2113.613	1371.001	1708.009	434.200	1983.090	-45.036
2400	1022.412	2157.029	1402.853	1810.023	435.925	2050.345	-44.624
2500	1026.579	2198.852	1433.862	1912.476	437.438	2117.648	-44.245
2600	1030.327	2239.190	1464.065	2015.324	438.703	2184.776	-43.892
2700	1033.711	2278.139	1493.498	2118.529	439.724	2251.934	-43.565
2800	1036.774	2315.789	1522.197	2222.056	440.474	2319.082	-43.262
2900	1039.555	2352.220	1550.194	2325.875	440.925	2386.153	-42.978
3000	1042.086	2387.506	1577.519	2429.959	441.121	2453.240	-42.714
3100	1044.397	2421.714	1604.203	2534.285	440.983	2520.247	-42.465
3200	1046.511	2454.906	1630.271	2638.831	440.554	2587.338	-42.233
3300	1048.449	2487.139	1655.751	2743.581	439.815	2654.489	-42.016
3400	1050.231	2518.465	1680.666	2848.516	438.739	2721.577	-41.811
3500	1051.873	2548.933	1705.041	2953.622	437.329	2788.683	-41.618
3600	1053.387	2578.586	1728.896	3058.886	435.609	2855.924	-41.438
3700	1054.788	2607.467	1752.252	3164.296	433.547	2923.234	-41.268
3800	1056.086	2635.614	1775.130	3269.841	431.115	2990.544	-41.107
3900	1057.291	2663.062	1797.547	3375.510	428.357	3057.868	-40.955
4000	1058.411	2689.845	1819.521	3481.296	425.255	3125.411	-40.813
4100	1059.455	2715.993	1841.068	3587.190	421.772	3192.959	-40.678
4200	1060.428	2741.535	1862.205	3693.185	417.939	3260.588	-40.551
4300	1061.337	2766.498	1882.946	3799.273	413.740	3328.219	-40.429
4400	1062.187	2790.908	1903.305	3905.450	409.184	3396.047	-40.315
4500	1062.983	2814.787	1923.296	4011.709	404.287	3464.040	-40.209
4600	1063.730	2838.158	1942.931	4118.045	398.996	3532.155	-40.108
4700	1064.432	2861.043	1962.223	4224.454	393.324	3600.271	-40.012
4800	1065.092	2883.460	1981.183	4330.930	387.321	3668.621	-39.922
4900	1065.714	2905.428	1999.821	4437.471	380.909	3736.960	-39.836
5000	1066.299	2926.964	2018.150	4544.072	374.186	3805.627	-39.756

3.368. Naphtho[2,1,8-*uva*]pentacene



Formula: $C_{28}H_{16}$
Mass: 352.427 g/mol
CAS Number: 196-45-2
Point Group: C_s

Length: 18.41 Å
Width: 9.620 Å
Breadth: 3.885 Å
L/B Ratio: 1.913

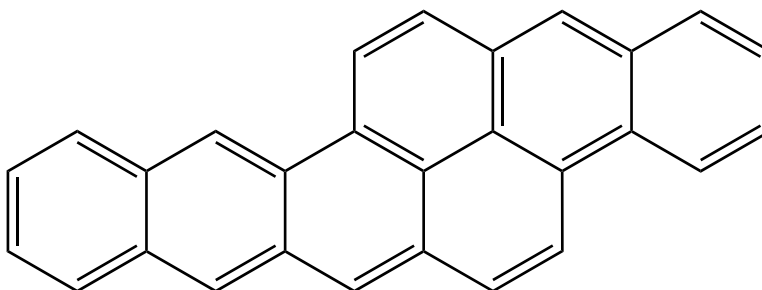
Cartesian coordinates:

C	7.1219	-1.1976	0.0000	C	-2.2829	1.6942	0.0000	H	6.4335	2.1581	0.0000
C	7.3335	0.2167	0.0000	C	-3.4299	2.5832	0.0000	H	5.6933	-2.7907	0.0000
C	6.2815	1.0728	0.0000	C	-4.6895	2.1091	0.0000	H	4.0045	2.5221	0.0000
C	5.8655	-1.7084	0.0000	C	-4.9583	0.6850	0.0000	H	3.2638	-2.4279	0.0000
C	4.7202	-0.8381	0.0000	C	-6.2528	0.1927	0.0000	H	1.5783	2.8809	0.0000
C	4.9316	0.5756	0.0000	C	-6.4843	-1.1913	0.0000	H	0.8295	-2.0652	0.0000
C	3.8459	1.4366	0.0000	C	-5.4329	-2.0803	0.0000	H	-0.8201	3.2595	0.0000
C	3.4299	-1.3436	0.0000	C	-3.8614	-0.2192	0.0000	H	-3.2329	3.6617	0.0000
C	2.3187	-0.4755	0.0000	C	-4.1022	-1.6079	0.0000	H	-5.5503	2.7878	0.0000
C	2.5289	0.9318	0.0000	C	-2.9905	-2.5042	0.0000	H	-7.1035	0.8835	0.0000
C	1.4117	1.7964	0.0000	C	-1.7157	-2.0263	0.0000	H	-7.5155	-1.5602	0.0000
C	0.9976	-0.9761	0.0000	C	-1.4511	-0.6238	0.0000	H	-5.6163	-3.1606	0.0000
C	-0.0914	-0.1238	0.0000	C	-2.5179	0.2697	0.0000	H	-3.1863	-3.5825	0.0000
C	0.1222	1.2924	0.0000	H	7.9967	-1.8561	0.0000	H	-0.8523	-2.7096	0.0000
C	-1.0082	2.1784	0.0000	H	8.3627	0.5904	0.0000				

Table 3.368: Table of thermodynamic data as a function of temperature for Naphtho[2,1,8-*uva*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-51.922	473.623	473.623	∞
100	112.103	359.109	808.713	-44.960	500.155	547.491	-285.974
200	225.029	469.508	611.449	-28.388	486.047	600.464	-156.822
250	290.371	526.696	588.749	-15.513	479.466	629.830	-131.593
298.15	353.810	583.280	583.280	0.000	473.623	659.335	-115.510
300	356.215	585.476	583.287	0.657	473.408	660.486	-114.998
350	419.381	645.180	587.858	20.063	468.034	692.103	-103.289
400	477.903	705.060	598.768	42.517	463.376	724.429	-94.599
450	530.906	764.464	613.885	67.761	459.348	757.307	-87.904
500	578.291	822.902	631.875	95.514	455.861	790.626	-82.594
600	657.784	935.650	673.192	157.475	450.206	858.140	-74.706
700	720.681	1041.956	718.359	226.518	446.101	926.481	-69.133
800	771.137	1141.602	765.105	301.198	443.369	995.297	-64.985
900	812.252	1234.882	812.177	380.435	441.834	1064.376	-61.774
1000	846.208	1322.274	858.864	463.410	441.334	1133.583	-59.211
1100	874.552	1404.296	904.759	549.490	441.669	1202.808	-57.115
1200	898.415	1481.444	949.634	638.172	442.699	1271.952	-55.365
1300	918.651	1554.176	993.367	729.052	444.240	1341.000	-53.881
1400	935.920	1622.904	1035.904	821.803	446.159	1409.918	-52.604
1500	950.742	1687.994	1077.224	916.155	448.374	1478.691	-51.492
1600	963.534	1749.772	1117.345	1011.884	450.756	1547.299	-50.513
1700	974.629	1808.527	1156.288	1108.805	453.229	1615.732	-49.644
1800	984.300	1864.515	1194.091	1206.762	455.718	1684.083	-48.870
1900	992.769	1917.965	1230.794	1305.625	458.193	1752.242	-48.172
2000	1000.218	1969.081	1266.440	1405.282	460.598	1820.300	-47.540
2100	1006.798	2018.044	1301.073	1505.640	462.855	1888.226	-46.966
2200	1012.634	2065.018	1334.737	1606.617	464.965	1956.050	-46.442
2300	1017.830	2110.148	1367.476	1708.145	466.921	2023.781	-45.961
2400	1022.473	2153.567	1399.331	1810.165	468.652	2091.382	-45.517
2500	1026.636	2195.392	1430.342	1912.624	470.172	2159.032	-45.110
2600	1030.382	2235.731	1460.548	2015.478	471.442	2226.505	-44.730
2700	1033.763	2274.683	1489.984	2118.688	472.468	2294.010	-44.379
2800	1036.823	2312.335	1518.685	2222.220	473.224	2361.503	-44.053
2900	1039.602	2348.767	1546.683	2326.044	473.679	2428.919	-43.749
3000	1042.131	2384.055	1574.011	2430.132	473.880	2496.351	-43.464
3100	1044.439	2418.264	1600.696	2534.462	473.746	2563.703	-43.197
3200	1046.551	2451.458	1626.766	2639.013	473.321	2631.140	-42.948
3300	1048.488	2483.692	1652.247	2743.767	472.586	2698.635	-42.715
3400	1050.268	2515.019	1677.165	2848.706	471.513	2766.067	-42.495
3500	1051.907	2545.488	1701.540	2953.816	470.107	2833.518	-42.287
3600	1053.421	2575.142	1725.397	3059.083	468.390	2901.103	-42.093
3700	1054.820	2604.024	1748.755	3164.496	466.331	2968.758	-41.910
3800	1056.117	2632.172	1771.634	3270.044	463.903	3036.412	-41.738
3900	1057.320	2659.621	1794.053	3375.716	461.148	3104.080	-41.574
4000	1058.439	2686.404	1816.028	3481.505	458.048	3171.967	-41.421
4100	1059.481	2712.553	1837.577	3587.401	454.569	3239.860	-41.275
4200	1060.453	2738.096	1858.715	3693.399	450.738	3307.832	-41.138
4300	1061.361	2763.059	1879.457	3799.490	446.541	3375.808	-41.007
4400	1062.210	2787.469	1899.817	3905.669	441.988	3443.980	-40.884
4500	1063.006	2811.349	1919.809	4011.930	437.094	3512.316	-40.769
4600	1063.752	2834.721	1939.445	4118.268	431.804	3580.775	-40.660
4700	1064.453	2857.606	1958.738	4224.679	426.135	3649.235	-40.556
4800	1065.112	2880.023	1977.699	4331.158	420.133	3717.928	-40.458
4900	1065.733	2901.992	1996.339	4437.700	413.724	3786.611	-40.365
5000	1066.318	2923.528	2014.668	4544.303	407.002	3855.621	-40.279

3.369. Anthra[2,1,9-*gra*]naphthacene



Formula: $C_{28}H_{16}$
Mass: 352.427 g/mol
CAS Number: 189-52-6
Point Group: C_s

Length: 18.40 Å
Width: 9.545 Å
Breadth: 3.886 Å
L/B Ratio: 1.928

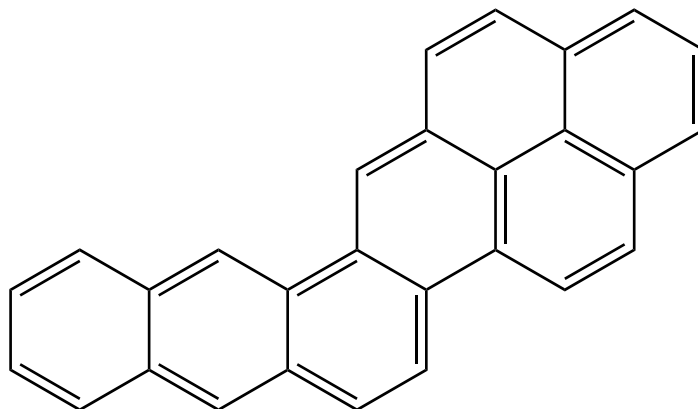
Cartesian coordinates:

C	6.7811	-1.2120	0.0000	C	-3.3777	-1.9544	0.0000	H	6.2683	2.1731	0.0000
C	7.0667	0.1855	0.0000	C	-1.7503	-0.1457	0.0000	H	5.2666	-2.7267	0.0000
C	6.0589	1.0974	0.0000	C	-2.0566	-1.5374	0.0000	H	3.8587	2.6620	0.0000
C	5.4961	-1.6552	0.0000	C	-0.9733	-2.4853	0.0000	H	2.8516	-2.2357	0.0000
C	4.4052	-0.7244	0.0000	C	0.3145	-2.0696	0.0000	H	1.4805	3.1635	0.0000
C	4.6899	0.6694	0.0000	C	0.6493	-0.6721	0.0000	H	-0.9121	3.6883	0.0000
C	3.6408	1.5867	0.0000	C	-0.3747	0.2720	0.0000	H	-3.2778	2.9236	0.0000
C	3.0805	-1.1578	0.0000	C	-4.4256	-1.0133	0.0000	H	-3.6166	-3.0252	0.0000
C	2.0213	-0.2425	0.0000	C	-4.1362	0.3718	0.0000	H	-1.2212	-3.5529	0.0000
C	2.3088	1.1510	0.0000	C	-5.2212	1.2972	0.0000	H	1.1470	-2.7903	0.0000
C	1.2397	2.0930	0.0000	C	-6.5139	0.8602	0.0000	H	-4.9819	2.3716	0.0000
C	-0.0672	1.6743	0.0000	C	-6.8013	-0.5287	0.0000	H	-7.3441	1.5740	0.0000
C	-1.1600	2.6206	0.0000	C	-5.7872	-1.4416	0.0000	H	-7.8467	-0.8540	0.0000
C	-2.4434	2.2053	0.0000	H	7.6179	-1.9180	0.0000	H	-5.9988	-2.5169	0.0000
C	-2.7824	0.8024	0.0000	H	8.1136	0.5064	0.0000				

Table 3.369: Table of thermodynamic data as a function of temperature for Anthra[2,1,9-*gra*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.669	468.804	468.804	∞
100	111.992	355.260	803.168	-44.791	495.505	543.227	-283.747
200	224.147	465.408	606.705	-28.260	481.357	596.594	-155.811
250	289.030	522.347	584.110	-15.441	474.720	626.171	-130.829
298.15	352.161	578.667	578.667	0.000	468.804	655.891	-114.907
300	354.556	580.853	578.674	0.654	468.586	657.051	-114.400
350	417.543	640.286	583.224	19.972	463.124	688.906	-102.811
400	475.995	699.914	594.085	42.332	458.372	721.483	-94.214
450	529.002	759.094	609.138	67.480	454.248	754.624	-87.593
500	576.437	817.333	627.055	95.139	450.667	788.217	-82.343
600	656.091	929.757	668.220	156.923	444.835	856.305	-74.546
700	719.166	1035.815	713.236	225.805	440.569	925.247	-69.041
800	769.786	1135.270	759.843	300.342	437.694	994.688	-64.945
900	811.044	1228.400	806.787	379.451	436.031	1064.408	-61.775
1000	845.125	1315.671	853.359	462.312	435.416	1134.270	-59.247
1100	873.577	1397.594	899.149	548.289	435.649	1204.160	-57.180
1200	897.534	1474.661	943.930	636.878	436.586	1273.978	-55.454
1300	917.853	1547.327	987.577	727.675	438.043	1343.708	-53.990
1400	935.195	1615.998	1030.034	820.349	439.886	1413.314	-52.730
1500	950.082	1681.040	1071.286	914.632	442.032	1482.780	-51.634
1600	962.930	1742.777	1111.341	1010.298	444.350	1552.086	-50.669
1700	974.076	1801.497	1150.226	1107.161	446.766	1621.219	-49.813
1800	983.793	1857.455	1187.974	1205.066	449.202	1690.275	-49.049
1900	992.302	1910.879	1224.626	1303.880	451.628	1759.142	-48.361
2000	999.787	1961.972	1260.226	1403.492	453.988	1827.909	-47.739
2100	1006.400	2010.915	1294.816	1503.808	456.204	1896.547	-47.173
2200	1012.265	2057.870	1328.440	1604.747	458.275	1965.085	-46.656
2300	1017.487	2102.985	1361.142	1706.240	460.196	2033.532	-46.182
2400	1022.153	2146.389	1392.962	1808.226	461.894	2101.850	-45.745
2500	1026.338	2188.202	1423.940	1910.654	463.382	2170.218	-45.343
2600	1030.103	2228.530	1454.115	2013.479	464.624	2238.411	-44.969
2700	1033.502	2267.471	1483.522	2116.663	465.623	2306.636	-44.624
2800	1036.578	2305.114	1512.196	2220.169	466.353	2374.850	-44.302
2900	1039.371	2341.538	1540.170	2323.969	466.785	2442.989	-44.002
3000	1041.914	2376.818	1567.473	2428.035	466.963	2511.145	-43.722
3100	1044.235	2411.021	1594.136	2532.344	466.808	2579.221	-43.459
3200	1046.358	2444.208	1620.184	2636.875	466.364	2647.382	-43.213
3300	1048.305	2476.436	1645.645	2741.610	465.610	2715.602	-42.984
3400	1050.095	2507.758	1670.543	2846.531	464.519	2783.761	-42.766
3500	1051.743	2538.222	1694.901	2951.624	463.096	2851.938	-42.562
3600	1053.265	2567.872	1718.740	3056.875	461.364	2920.250	-42.371
3700	1054.672	2596.750	1742.081	3162.273	459.290	2988.632	-42.191
3800	1055.976	2624.894	1764.945	3267.806	456.847	3057.013	-42.021
3900	1057.186	2652.339	1787.348	3373.465	454.078	3125.410	-41.859
4000	1058.311	2679.119	1809.309	3479.241	450.965	3194.025	-41.709
4100	1059.359	2705.265	1830.844	3585.125	447.473	3262.646	-41.566
4200	1060.336	2730.804	1851.969	3691.110	443.631	3331.348	-41.431
4300	1061.249	2755.765	1872.698	3797.190	439.422	3400.052	-41.302
4400	1062.103	2780.173	1893.046	3903.358	434.858	3468.954	-41.181
4500	1062.903	2804.050	1913.026	4009.609	429.953	3538.020	-41.067
4600	1063.654	2827.420	1932.651	4115.937	424.654	3607.209	-40.960
4700	1064.359	2850.303	1951.933	4222.338	418.975	3676.399	-40.858
4800	1065.022	2872.718	1970.883	4328.808	412.964	3745.823	-40.762
4900	1065.646	2894.685	1989.513	4435.341	406.546	3815.236	-40.670
5000	1066.234	2916.220	2007.833	4541.936	399.816	3884.977	-40.585

3.370. Naphtho[8,1,2-*cde*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-50-9
Point Group: C_s

Length: 18.01 Å
Width: 9.200 Å
Breadth: 3.885 Å
L/B Ratio: 1.958

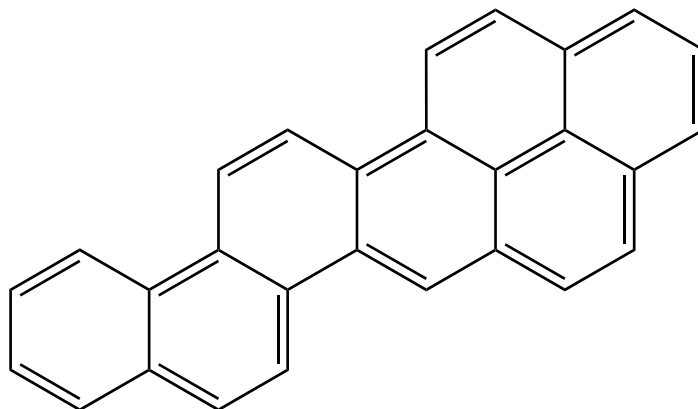
Cartesian coordinates:

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C	7.0005	-0.5824	0.0000	C	-3.4606	-2.6892	0.0000	H	4.5720	-2.9909	0.0000
C	6.2281	0.5414	0.0000	C	-2.1139	-2.5865	0.0000	H	4.4507	2.5752	0.0000
C	5.0431	-2.0015	0.0000	C	-4.2978	-1.5135	0.0000	H	2.3375	-1.9540	0.0000
C	4.2060	-0.8446	0.0000	C	-5.8827	0.8009	0.0000	H	2.2521	3.6160	0.0000
C	4.8039	0.4381	0.0000	C	-6.4710	-0.4545	0.0000	H	-0.2228	3.4210	0.0000
C	3.9856	1.5816	0.0000	C	-5.6891	-1.6076	0.0000	H	0.5499	-2.0917	0.0000
C	2.8046	-0.9560	0.0000	C	-2.2578	-0.1229	0.0000	H	-3.9529	-3.6685	0.0000
C	1.9975	0.1727	0.0000	C	-1.6494	1.1456	0.0000	H	-1.4797	-3.4805	0.0000
C	2.6035	1.4611	0.0000	C	-2.4922	2.3117	0.0000	H	-6.5057	1.7025	0.0000
C	1.7643	2.6343	0.0000	C	-3.8425	2.2103	0.0000	H	-7.5626	-0.5431	0.0000
C	0.4195	2.5269	0.0000	C	-4.4868	0.9254	0.0000	H	-6.1679	-2.5933	0.0000
C	0.5453	0.0713	0.0000	C	-3.6864	-0.2371	0.0000	H	-1.9972	3.2949	0.0000
C	-0.2347	1.2419	0.0000	H	7.0470	-2.7537	0.0000	H	-4.4748	3.1056	0.0000
C	-0.0797	-1.1872	0.0000	H	8.0930	-0.5092	0.0000				

Table 3.370: Table of thermodynamic data as a function of temperature for Naphtho[8,1,2-*cde*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-51.620	444.069	444.069	∞
100	111.656	358.494	805.317	-44.682	470.878	518.276	-270.714
200	223.571	468.292	609.305	-28.203	456.678	571.338	-149.215
250	288.449	525.103	586.754	-15.413	450.012	600.774	-125.522
298.15	351.581	581.320	581.320	0.000	444.069	630.365	-110.435
300	353.976	583.502	581.327	0.653	443.849	631.519	-109.955
350	416.975	642.847	585.870	19.942	438.359	663.244	-98.982
400	475.447	702.401	596.715	42.274	433.579	695.695	-90.847
450	528.482	761.517	611.749	67.396	429.428	728.714	-84.585
500	575.948	819.703	629.645	95.029	425.822	762.186	-79.623
600	655.667	932.044	670.765	156.767	419.944	830.042	-72.260
700	718.802	1038.041	715.741	225.610	415.639	898.759	-67.065
800	769.472	1137.451	762.309	300.113	412.730	967.979	-63.201
900	810.773	1230.546	809.220	379.194	411.038	1037.483	-60.213
1000	844.889	1317.791	855.761	462.029	410.398	1107.131	-57.829
1100	873.370	1399.693	901.525	547.984	410.609	1176.811	-55.881
1200	897.352	1476.743	946.282	636.554	411.526	1246.420	-54.254
1300	917.691	1549.395	989.908	727.333	412.966	1315.942	-52.874
1400	935.051	1618.055	1032.346	819.993	414.793	1385.342	-51.687
1500	949.952	1683.088	1073.580	914.261	416.926	1454.603	-50.653
1600	962.814	1744.817	1113.620	1009.915	419.232	1523.704	-49.743
1700	973.971	1803.530	1152.490	1106.767	421.636	1592.634	-48.935
1800	983.697	1859.482	1190.225	1204.662	424.063	1661.487	-48.214
1900	992.215	1912.901	1226.866	1303.467	426.479	1730.151	-47.564
2000	999.707	1963.989	1262.454	1403.071	428.831	1798.717	-46.977
2100	1006.326	2012.929	1297.034	1503.379	431.040	1867.153	-46.442
2200	1012.197	2059.881	1330.649	1604.311	433.104	1935.490	-45.953
2300	1017.424	2104.993	1363.342	1705.797	435.018	2003.736	-45.505
2400	1022.095	2148.394	1395.154	1807.777	436.710	2071.853	-45.092
2500	1026.284	2190.205	1426.125	1910.200	438.193	2140.021	-44.712
2600	1030.053	2230.531	1456.293	2013.020	439.429	2208.014	-44.359
2700	1033.455	2269.471	1485.693	2116.198	440.423	2276.038	-44.032
2800	1036.535	2307.111	1514.361	2219.700	441.149	2344.053	-43.728
2900	1039.330	2343.534	1542.329	2323.496	441.577	2411.992	-43.444
3000	1041.876	2378.813	1569.627	2427.558	441.751	2479.948	-43.179
3100	1044.198	2413.014	1596.284	2531.864	441.592	2547.825	-42.930
3200	1046.324	2446.200	1622.328	2636.391	441.144	2615.787	-42.697
3300	1048.273	2478.428	1647.784	2741.123	440.387	2683.808	-42.480
3400	1050.064	2509.749	1672.678	2846.041	439.293	2751.767	-42.275
3500	1051.715	2540.212	1697.031	2951.131	437.867	2819.745	-42.082
3600	1053.238	2569.861	1720.867	3056.379	436.132	2887.858	-41.901
3700	1054.646	2598.738	1744.204	3161.774	434.055	2956.042	-41.731
3800	1055.951	2626.881	1767.064	3267.305	431.610	3024.224	-41.570
3900	1057.163	2654.326	1789.464	3372.962	428.838	3092.422	-41.417
4000	1058.289	2681.105	1811.422	3478.735	425.724	3160.839	-41.275
4100	1059.338	2707.250	1832.953	3584.617	422.230	3229.261	-41.140
4200	1060.316	2732.790	1854.075	3690.600	418.385	3297.764	-41.013
4300	1061.230	2757.750	1874.802	3796.678	414.175	3366.270	-40.891
4400	1062.085	2782.157	1895.147	3902.844	409.609	3434.973	-40.777
4500	1062.886	2806.034	1915.125	4009.093	404.702	3503.841	-40.671
4600	1063.637	2829.404	1934.747	4115.420	399.400	3572.831	-40.570
4700	1064.343	2852.286	1954.027	4221.819	393.720	3641.823	-40.473
4800	1065.006	2874.701	1972.975	4328.287	387.707	3711.049	-40.384
4900	1065.631	2896.667	1991.602	4434.819	381.288	3780.264	-40.297
5000	1066.220	2918.202	2009.920	4541.412	374.556	3849.807	-40.218

3.371. Dibenzo[*c,pqr*]picene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-44-1
Point Group: C_s

Length: 18.02 Å
Width: 9.197 Å
Breadth: 3.886 Å
L/B Ratio: 1.959

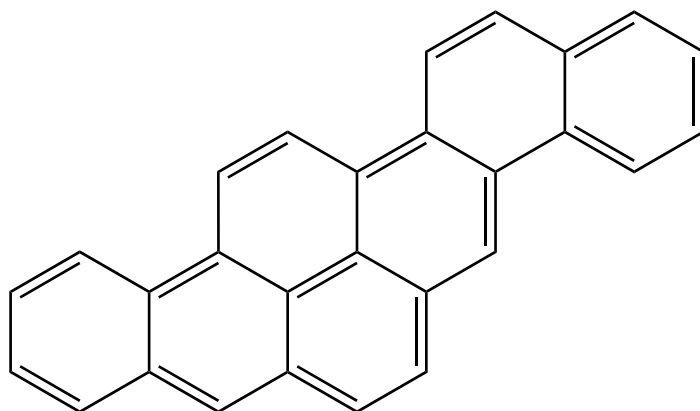
Cartesian coordinates:

C	5.9294	-0.9699	0.0000	C	0.0470	0.8451	0.0000	H	6.1356	2.4343	0.0000
C	6.4912	0.3081	0.0000	C	-0.8225	1.9788	0.0000	H	2.1323	-3.5763	0.0000
C	5.6873	1.4344	0.0000	C	-2.1722	1.8267	0.0000	H	4.5974	-3.3111	0.0000
C	4.5467	-1.1286	0.0000	C	-1.9447	-0.6021	0.0000	H	-0.1114	-2.5806	0.0000
C	2.5933	-2.5818	0.0000	C	-2.7653	0.5275	0.0000	H	3.8834	3.4457	0.0000
C	3.9348	-2.4379	0.0000	C	-3.8913	-2.0573	0.0000	H	1.4103	3.1803	0.0000
C	1.7139	-1.4334	0.0000	C	-2.5421	-1.9021	0.0000	H	-0.3637	2.9795	0.0000
C	0.3420	-1.5765	0.0000	C	-4.7547	-0.9175	0.0000	H	-2.8433	2.6994	0.0000
C	3.7130	0.0168	0.0000	C	-4.1981	0.3745	0.0000	H	-4.3427	-3.0561	0.0000
C	4.2890	1.3044	0.0000	C	-5.0667	1.4924	0.0000	H	-1.8741	-2.7769	0.0000
C	3.4249	2.4503	0.0000	C	-6.4288	1.3211	0.0000	H	-4.6226	2.4995	0.0000
C	2.0768	2.3041	0.0000	C	-6.9818	0.0259	0.0000	H	-7.0956	2.1895	0.0000
C	1.4641	1.0056	0.0000	C	-6.1612	-1.0750	0.0000	H	-8.0702	-0.0931	0.0000
C	2.2879	-0.1282	0.0000	H	6.5800	-1.8518	0.0000	H	-6.5833	-2.0864	0.0000
C	-0.5108	-0.4483	0.0000	H	7.5810	0.4166	0.0000				

Table 3.371: Table of thermodynamic data as a function of temperature for Dibenzo[*c,pqr*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-51.805	437.553	437.553	∞
100	112.632	361.522	809.097	-44.757	464.288	511.383	-267.114
200	223.898	471.757	612.850	-28.218	450.147	564.114	-147.328
250	288.600	528.621	590.288	-15.417	443.492	593.375	-123.976
298.15	351.608	584.854	584.854	0.000	437.553	622.796	-109.109
300	354.000	587.036	584.860	0.653	437.334	623.944	-108.636
350	416.918	646.378	589.403	19.941	431.842	655.492	-97.825
400	475.344	705.920	600.248	42.269	427.058	687.767	-89.811
450	528.353	765.023	615.279	67.385	422.902	720.610	-83.644
500	575.805	823.195	633.172	95.011	419.289	753.907	-78.759
600	655.503	935.508	674.284	156.734	413.395	821.415	-71.509
700	718.617	1041.478	719.250	225.560	409.073	889.787	-66.395
800	769.267	1140.861	765.807	300.043	406.145	958.665	-62.593
900	810.552	1233.932	812.707	379.102	404.431	1027.829	-59.652
1000	844.657	1321.152	859.237	461.915	403.768	1097.140	-57.308
1100	873.134	1403.032	904.990	547.846	403.956	1166.484	-55.391
1200	897.116	1480.062	949.735	636.392	404.850	1235.761	-53.790
1300	917.460	1552.695	993.350	727.148	406.266	1304.952	-52.433
1400	934.826	1621.338	1035.777	819.785	408.070	1374.023	-51.264
1500	949.737	1686.356	1077.001	914.032	410.181	1442.956	-50.247
1600	962.608	1748.071	1117.031	1009.665	412.466	1511.731	-49.352
1700	973.775	1806.772	1155.891	1106.497	414.850	1580.337	-48.557
1800	983.512	1862.713	1193.617	1204.372	417.257	1648.866	-47.848
1900	992.040	1916.122	1230.249	1303.159	419.656	1717.207	-47.208
2000	999.542	1967.202	1265.829	1402.746	421.991	1785.451	-46.630
2100	1006.171	2016.134	1300.401	1503.038	424.183	1853.566	-46.104
2200	1012.050	2063.079	1334.009	1603.955	426.232	1921.583	-45.623
2300	1017.286	2108.184	1366.694	1705.427	428.132	1989.510	-45.182
2400	1021.965	2151.580	1398.499	1807.394	429.811	2057.308	-44.775
2500	1026.161	2193.385	1429.464	1909.804	431.281	2125.158	-44.402
2600	1029.937	2233.707	1459.626	2012.612	432.505	2192.833	-44.054
2700	1033.345	2272.642	1489.020	2115.779	433.488	2260.540	-43.732
2800	1036.431	2310.279	1517.683	2219.270	434.203	2328.238	-43.433
2900	1039.232	2346.698	1545.645	2323.055	434.621	2395.860	-43.153
3000	1041.782	2381.974	1572.938	2427.108	434.785	2463.500	-42.892
3100	1044.110	2416.172	1599.590	2531.404	434.618	2531.061	-42.647
3200	1046.240	2449.355	1625.629	2635.923	434.161	2598.707	-42.419
3300	1048.193	2481.580	1651.081	2740.647	433.396	2666.413	-42.205
3400	1049.989	2512.899	1675.970	2845.557	432.294	2734.057	-42.003
3500	1051.642	2543.360	1700.320	2950.640	430.861	2801.720	-41.813
3600	1053.169	2573.007	1724.151	3055.881	429.118	2869.519	-41.635
3700	1054.581	2601.882	1747.485	3161.269	427.035	2937.387	-41.468
3800	1055.889	2630.024	1770.341	3266.794	424.583	3005.255	-41.309
3900	1057.103	2657.467	1792.738	3372.444	421.805	3073.139	-41.159
4000	1058.232	2684.245	1814.692	3478.212	418.685	3141.242	-41.020
4100	1059.283	2710.388	1836.221	3584.088	415.185	3209.350	-40.887
4200	1060.264	2735.926	1857.339	3690.066	411.335	3277.540	-40.761
4300	1061.180	2760.886	1878.063	3796.138	407.120	3345.732	-40.642
4400	1062.037	2785.292	1898.405	3902.300	402.549	3414.122	-40.530
4500	1062.839	2809.168	1918.380	4008.544	397.637	3482.676	-40.425
4600	1063.592	2832.536	1938.000	4114.866	392.331	3551.353	-40.326
4700	1064.300	2855.418	1957.277	4221.261	386.646	3620.032	-40.231
4800	1064.965	2877.832	1976.223	4327.725	380.630	3688.944	-40.143
4900	1065.591	2899.797	1994.848	4434.253	374.206	3757.846	-40.058
5000	1066.181	2921.331	2013.163	4540.842	367.471	3827.076	-39.980

3.372. Dibenzo[*c,rst*]pentaphene



Formula: C₂₈H₁₆
Mass: 352.427 g/mol
CAS Number: 120835-52-1
Point Group: C_s

Length: 18.02 Å
Width: 9.196 Å
Breadth: 3.884 Å
L/B Ratio: 1.960

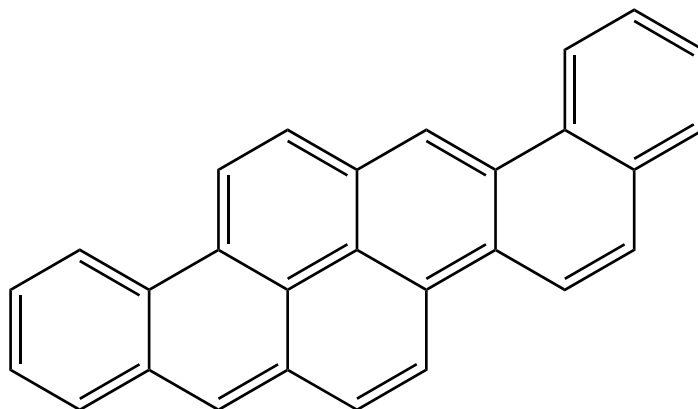
Cartesian coordinates:

C	6.0564	-1.7070	0.0000	C	-0.3851	-0.8637	0.0000	H	6.3931	1.6889	0.0000
C	6.6772	-0.4398	0.0000	C	0.4133	-2.0482	0.0000	H	4.1887	-2.7870	0.0000
C	5.9178	0.7014	0.0000	C	1.7720	-1.9803	0.0000	H	4.2157	2.7780	0.0000
C	4.6894	-1.8066	0.0000	C	-1.8136	-0.9206	0.0000	H	2.0387	3.8950	0.0000
C	3.8794	-0.6430	0.0000	C	-2.5563	0.2692	0.0000	H	-0.4353	3.7682	0.0000
C	4.5009	0.6217	0.0000	C	-3.8542	-2.2418	0.0000	H	-2.4943	2.4363	0.0000
C	3.7099	1.8044	0.0000	C	-2.4999	-2.1790	0.0000	H	-0.1054	-3.0190	0.0000
C	2.3394	1.7311	0.0000	C	-4.6404	-1.0438	0.0000	H	2.3891	-2.8922	0.0000
C	1.5221	2.9281	0.0000	C	-4.0004	0.2084	0.0000	H	-4.3737	-3.2069	0.0000
C	0.1776	2.8594	0.0000	C	-4.7919	1.3795	0.0000	H	-1.8884	-3.0945	0.0000
C	-0.5117	1.5851	0.0000	C	-6.1641	1.2987	0.0000	H	-4.2834	2.3557	0.0000
C	-1.8865	1.5170	0.0000	C	-6.8002	0.0445	0.0000	H	-6.7711	2.2100	0.0000
C	2.4467	-0.7226	0.0000	C	-6.0522	-1.1090	0.0000	H	-7.8940	-0.0042	0.0000
C	1.6882	0.4532	0.0000	H	6.6784	-2.6080	0.0000	H	-6.5406	-2.0900	0.0000
C	0.2597	0.3834	0.0000	H	7.7704	-0.3799	0.0000				

Table 3.372: Table of thermodynamic data as a function of temperature for Dibenzoc[*c,rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-51.765	440.485	440.485	∞
100	112.711	357.275	805.244	-44.797	467.180	514.700	-268.846
200	224.090	467.661	608.839	-28.236	453.062	567.848	-148.304
250	288.764	524.562	586.265	-15.426	446.416	597.313	-124.799
298.15	351.818	580.827	580.827	0.000	440.485	626.928	-109.833
300	354.213	583.011	580.834	0.653	440.266	628.084	-109.357
350	417.207	642.391	585.379	19.954	434.787	659.832	-98.473
400	475.702	701.977	596.231	42.298	430.019	692.306	-90.404
450	528.761	761.125	611.274	67.433	425.882	725.344	-84.194
500	576.241	819.341	629.179	95.081	422.290	758.836	-79.273
600	655.954	931.735	670.321	156.848	416.442	826.724	-71.971
700	719.054	1037.774	715.319	225.719	412.164	895.470	-66.819
800	769.678	1137.215	761.909	300.245	409.278	964.716	-62.988
900	810.934	1230.332	808.839	379.343	407.604	1034.242	-60.025
1000	845.011	1317.591	855.398	462.193	406.978	1103.911	-57.661
1100	873.460	1399.503	901.178	548.158	407.199	1173.610	-55.729
1200	897.416	1476.560	945.948	636.735	408.125	1243.238	-54.116
1300	917.735	1549.216	989.585	727.520	409.569	1312.778	-52.747
1400	935.080	1617.879	1032.034	820.183	411.401	1382.196	-51.569
1500	949.970	1682.913	1073.277	914.454	413.536	1451.474	-50.544
1600	962.823	1744.643	1113.325	1010.109	415.843	1520.593	-49.641
1700	973.974	1803.357	1152.202	1106.962	418.248	1589.540	-48.840
1800	983.695	1859.309	1189.944	1204.857	420.674	1658.410	-48.125
1900	992.209	1912.727	1226.590	1303.661	423.090	1727.092	-47.480
2000	999.699	1963.816	1262.183	1403.264	425.442	1795.674	-46.897
2100	1006.316	2012.754	1296.768	1503.572	427.649	1864.128	-46.367
2200	1012.186	2059.706	1330.387	1604.503	429.712	1932.482	-45.882
2300	1017.412	2104.817	1363.084	1705.987	431.625	2000.746	-45.437
2400	1022.083	2148.219	1394.899	1807.966	433.316	2068.881	-45.027
2500	1026.271	2190.028	1425.873	1910.388	434.797	2137.066	-44.651
2600	1030.040	2230.354	1456.044	2013.207	436.032	2205.077	-44.300
2700	1033.442	2269.293	1485.447	2116.384	437.025	2273.119	-43.975
2800	1036.522	2306.934	1514.118	2219.884	437.750	2341.152	-43.674
2900	1039.318	2343.356	1542.088	2323.679	438.176	2409.108	-43.392
3000	1041.863	2378.634	1569.388	2427.740	438.349	2477.083	-43.129
3100	1044.186	2412.835	1596.047	2532.044	438.189	2544.977	-42.882
3200	1046.312	2446.021	1622.092	2636.570	437.740	2612.957	-42.651
3300	1048.261	2478.248	1647.551	2741.300	436.982	2680.996	-42.436
3400	1050.053	2509.568	1672.446	2846.217	435.887	2748.973	-42.232
3500	1051.704	2540.031	1696.801	2951.306	434.459	2816.969	-42.040
3600	1053.227	2569.680	1720.637	3056.554	432.723	2885.101	-41.861
3700	1054.636	2598.557	1743.976	3161.948	430.645	2953.302	-41.692
3800	1055.942	2626.700	1766.837	3267.478	428.199	3021.502	-41.533
3900	1057.153	2654.144	1789.238	3373.133	425.426	3089.719	-41.381
4000	1058.280	2680.923	1811.197	3478.905	422.311	3158.153	-41.240
4100	1059.329	2707.068	1832.730	3584.786	418.816	3226.594	-41.106
4200	1060.307	2732.607	1853.853	3690.769	414.970	3295.115	-40.980
4300	1061.222	2757.568	1874.580	3796.846	410.759	3363.640	-40.859
4400	1062.077	2781.974	1894.926	3903.011	406.192	3432.361	-40.746
4500	1062.878	2805.851	1914.905	4009.259	401.285	3501.247	-40.641
4600	1063.629	2829.221	1934.528	4115.585	395.982	3570.256	-40.541
4700	1064.335	2852.103	1953.808	4221.984	390.301	3639.266	-40.445
4800	1064.999	2874.518	1972.757	4328.451	384.288	3708.510	-40.356
4900	1065.624	2896.484	1991.385	4434.982	377.867	3777.743	-40.270
5000	1066.213	2918.018	2009.703	4541.574	371.136	3847.304	-40.192

3.373. Dibenzo[*b,tuv*]picene



Other names: Benzo[*a*]naphtho[2,1-*h*]pyrene

Formula: C₂₈H₁₆

Mass: 352.427 g/mol

CAS Number: 189-18-4

Point Group: C_s

Length: 18.02 Å

Width: 9.197 Å

Breadth: 3.887 Å

L/B Ratio: 1.959

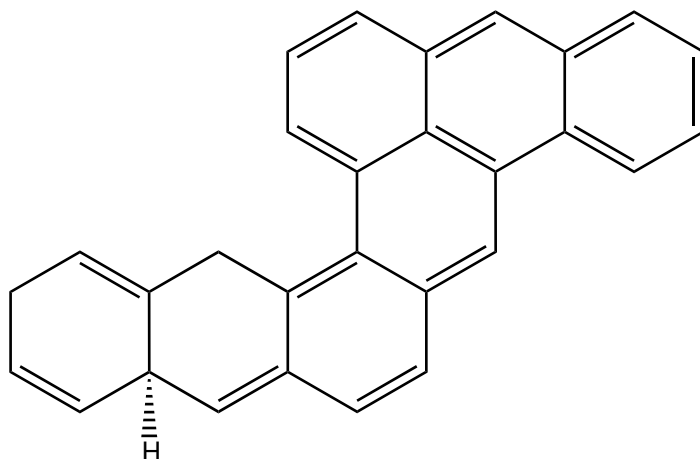
Cartesian coordinates:

C	6.2173	-1.5311	0.0000	C	-0.2680	-1.2304	0.0000	H	6.2782	1.8828	0.0000
C	6.7340	-0.2138	0.0000	C	0.6339	-2.3509	0.0000	H	4.4486	-2.7610	0.0000
C	5.8866	0.8591	0.0000	C	1.9745	-2.1635	0.0000	H	4.0175	2.7885	0.0000
C	4.8665	-1.7427	0.0000	C	-2.5184	-0.3152	0.0000	H	1.7455	3.7161	0.0000
C	3.9583	-0.6481	0.0000	C	-1.9966	0.9975	0.0000	H	-0.7123	3.3724	0.0000
C	4.4761	0.6656	0.0000	C	-2.9062	2.1120	0.0000	H	-2.0714	-2.4290	0.0000
C	3.5975	1.7750	0.0000	C	-4.2462	1.9296	0.0000	H	0.2055	-3.3597	0.0000
C	2.2311	1.5877	0.0000	C	-3.9556	-0.5106	0.0000	H	2.6717	-3.0157	0.0000
C	1.3183	2.7066	0.0000	C	-4.8079	0.6068	0.0000	H	-2.4713	3.1232	0.0000
C	-0.0180	2.5181	0.0000	C	-6.2060	0.4210	0.0000	H	-4.9324	2.7843	0.0000
C	-0.5961	1.1954	0.0000	C	-6.7381	-0.8493	0.0000	H	-6.8623	1.2987	0.0000
C	-1.6464	-1.4122	0.0000	C	-5.8905	-1.9679	0.0000	H	-7.8234	-0.9941	0.0000
C	2.5445	-0.8442	0.0000	C	-4.5235	-1.8018	0.0000	H	-6.3234	-2.9736	0.0000
C	1.6913	0.2651	0.0000	H	6.9129	-2.3765	0.0000	H	-3.8497	-2.6722	0.0000
C	0.2671	0.0836	0.0000	H	7.8191	-0.0674	0.0000				

Table 3.373: Table of thermodynamic data as a function of temperature for Dibenzo[*b,tuv*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-52.126	447.975	447.975	∞
100	113.905	361.655	811.904	-45.025	474.443	521.524	-272.411
200	225.260	472.853	614.586	-28.347	460.441	574.189	-149.960
250	289.899	530.013	591.927	-15.479	453.853	603.388	-126.068
298.15	352.880	586.472	586.472	0.000	447.975	632.736	-110.850
300	355.271	588.662	586.478	0.655	447.759	633.880	-110.366
350	418.168	648.198	591.037	20.006	442.330	665.342	-99.295
400	476.563	707.906	601.915	42.396	437.608	697.522	-91.085
450	529.526	767.150	616.990	67.572	433.511	730.262	-84.765
500	576.920	825.442	634.930	95.256	429.955	763.450	-79.755
600	656.489	937.947	676.141	157.083	424.167	830.723	-72.319
700	719.475	1044.059	721.200	226.001	419.937	898.844	-67.071
800	770.013	1143.550	767.844	300.565	417.088	967.458	-63.167
900	811.201	1236.702	814.821	379.693	415.445	1036.349	-60.147
1000	845.225	1323.987	861.420	462.567	414.842	1105.380	-57.738
1100	873.634	1405.917	907.234	548.551	415.083	1174.438	-55.768
1200	897.558	1482.988	952.035	637.145	416.024	1243.424	-54.124
1300	917.853	1555.655	995.699	727.942	417.482	1312.321	-52.729
1400	935.178	1624.325	1038.171	820.616	419.324	1381.094	-51.528
1500	950.053	1689.366	1079.435	914.896	421.468	1449.727	-50.483
1600	962.893	1751.101	1119.501	1010.559	423.783	1518.200	-49.563
1700	974.034	1809.818	1158.395	1107.418	426.194	1586.502	-48.746
1800	983.747	1865.773	1196.152	1205.318	428.626	1654.726	-48.018
1900	992.254	1919.195	1232.812	1304.128	431.047	1722.761	-47.361
2000	999.739	1970.285	1268.418	1403.735	433.403	1790.696	-46.767
2100	1006.351	2019.226	1303.013	1504.046	435.614	1858.503	-46.227
2200	1012.217	2066.179	1336.643	1604.981	437.680	1926.210	-45.733
2300	1017.440	2111.292	1369.349	1706.468	439.596	1993.826	-45.280
2400	1022.108	2154.694	1401.173	1808.450	441.289	2061.314	-44.862
2500	1026.294	2196.505	1432.155	1910.874	442.773	2128.851	-44.479
2600	1030.061	2236.831	1462.333	2013.695	444.010	2196.214	-44.122
2700	1033.460	2275.771	1491.744	2116.874	445.005	2263.609	-43.791
2800	1036.539	2313.412	1520.421	2220.376	445.732	2330.994	-43.484
2900	1039.333	2349.835	1548.397	2324.172	446.159	2398.303	-43.197
3000	1041.877	2385.114	1575.702	2428.234	446.334	2465.629	-42.930
3100	1044.199	2419.315	1602.367	2532.540	446.175	2532.875	-42.678
3200	1046.324	2452.501	1628.418	2637.068	445.727	2600.207	-42.443
3300	1048.273	2484.729	1653.880	2741.799	444.970	2667.598	-42.224
3400	1050.064	2516.050	1678.780	2846.717	443.876	2734.927	-42.016
3500	1051.714	2546.512	1703.139	2951.807	442.450	2802.275	-41.821
3600	1053.236	2576.162	1726.980	3057.056	440.715	2869.758	-41.638
3700	1054.645	2605.039	1750.322	3162.450	438.638	2937.311	-41.467
3800	1055.950	2633.182	1773.187	3267.981	436.192	3004.864	-41.304
3900	1057.161	2660.627	1795.591	3373.637	433.421	3072.432	-41.150
4000	1058.287	2687.406	1817.553	3479.410	430.306	3140.218	-41.006
4100	1059.336	2713.551	1839.089	3585.292	426.812	3208.010	-40.870
4200	1060.314	2739.090	1860.215	3691.275	422.967	3275.883	-40.741
4300	1061.228	2764.051	1880.945	3797.353	418.756	3343.760	-40.618
4400	1062.083	2788.458	1901.294	3903.519	414.190	3411.832	-40.503
4500	1062.883	2812.335	1921.275	4009.767	409.283	3480.070	-40.395
4600	1063.635	2835.704	1940.901	4116.094	403.981	3548.430	-40.293
4700	1064.340	2858.586	1960.184	4222.493	398.300	3616.792	-40.195
4800	1065.004	2881.001	1979.135	4328.960	392.288	3685.388	-40.104
4900	1065.628	2902.968	1997.765	4435.492	385.868	3753.973	-40.017
5000	1066.217	2924.502	2016.085	4542.085	379.136	3822.886	-39.937

3.374. 1*H*-Dibenzo[*a,de*]naphth[2,3-*h*]anthracene



Other names: 1*H*-Dibenzo[*c,uv*]pentaphene

Formula: C₂₉H₁₈

Mass: 366.453 g/mol

CAS Number: 195-85-7

Point Group: C₁

Length: 17.49 Å

Width: 10.32 Å

Breadth: 6.101 Å

L/B Ratio: 1.695

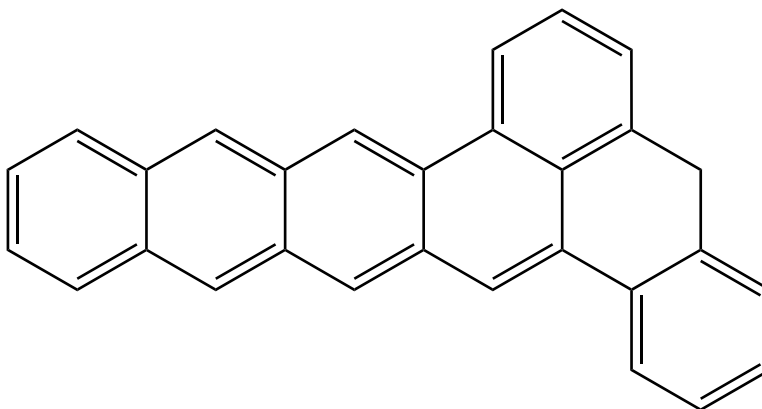
Cartesian coordinates:

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C	-2.5330	1.9386	0.2181	C	2.6167	0.8143	0.1941	H	4.3296	-2.7740	0.1616
C	-1.7584	0.7512	0.3315	C	5.9144	-0.8163	-0.7523	H	2.0762	1.4528	-0.5404
C	-0.3661	0.8405	0.7008	C	6.6403	0.2872	-1.1711	H	2.6628	1.4119	1.1356
C	0.1202	2.0542	1.1203	C	6.0591	1.5549	-1.1515	H	2.3545	-3.7906	1.0804
C	-0.6716	3.2326	1.0581	C	4.7533	1.7166	-0.7126	H	-0.1296	-3.7450	1.2539
C	-2.3752	-0.4954	0.1328	C	-3.8609	1.8687	-0.2008	H	-2.1591	-2.6473	0.3914
C	-1.6165	-1.6885	0.4133	C	-4.4598	0.6320	-0.4694	H	-2.5463	4.1029	0.4889
C	-0.2909	-1.6348	0.6889	C	-3.7255	-0.5663	-0.2786	H	-0.2259	4.1780	1.3850
C	0.4510	-0.3750	0.6337	C	-4.3817	-1.8150	-0.5090	H	1.1353	2.1487	1.5321
C	0.4443	-2.8543	0.9745	C	-5.6776	-1.8573	-0.9258	H	-4.4469	2.7898	-0.3089
C	1.7816	-2.8785	0.8772	C	-6.4057	-0.6541	-1.1362	H	-3.8042	-2.7362	-0.3369
C	2.5161	-1.6901	0.4730	C	-5.8185	0.5539	-0.9125	H	-6.1763	-2.8152	-1.1057
C	1.8071	-0.4136	0.4487	H	6.6356	2.4242	-1.4842	H	-7.4441	-0.7183	-1.4772
C	3.8218	-1.8014	0.1276	H	7.6713	0.1655	-1.5187	H	-6.3721	1.4872	-1.0660
C	4.5937	-0.6609	-0.3088	H	6.3675	-1.8140	-0.7670				

Table 3.374: Table of thermodynamic data as a function of temperature for 1*H*-Dibenzo[*a,de*]naphth[2,3-*h*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.434	568.530	568.530	∞
100	121.197	369.616	849.775	-48.016	598.465	654.919	-342.088
200	240.419	488.407	639.394	-30.197	582.584	717.720	-187.445
250	308.802	549.349	615.263	-16.479	575.155	752.364	-157.195
298.15	375.520	609.456	609.456	0.000	568.530	787.111	-137.896
300	378.055	611.787	609.463	0.697	568.286	788.466	-137.281
350	444.794	675.125	614.313	21.284	562.174	825.660	-123.220
400	506.824	738.628	625.885	45.097	556.866	863.663	-112.780
450	563.130	801.633	641.920	71.871	552.278	902.293	-104.733
500	613.553	863.625	661.001	101.312	548.319	941.422	-98.348
600	698.322	983.284	704.831	167.072	541.956	1020.676	-88.856
700	765.585	1096.177	752.758	240.393	537.419	1100.852	-82.145
800	819.701	1202.065	802.375	319.752	534.491	1181.548	-77.146
900	863.921	1301.250	852.355	404.005	532.963	1262.520	-73.273
1000	900.533	1394.226	901.943	492.283	532.639	1343.609	-70.181
1100	931.159	1481.535	950.706	583.912	533.291	1424.692	-67.652
1200	956.989	1563.695	998.399	678.355	534.753	1505.660	-65.538
1300	978.925	1641.185	1044.892	775.180	536.818	1586.492	-63.745
1400	997.667	1714.435	1090.124	874.034	539.335	1667.151	-62.201
1500	1013.771	1783.829	1134.079	974.626	542.209	1747.619	-60.856
1600	1027.679	1849.711	1176.764	1076.715	545.295	1827.878	-59.673
1700	1039.752	1912.385	1218.208	1180.101	548.506	1907.913	-58.622
1800	1050.281	1972.120	1258.446	1284.614	551.761	1987.827	-57.684
1900	1059.506	2029.158	1297.520	1390.114	555.021	2067.504	-56.838
2000	1067.624	2083.715	1335.476	1496.479	558.225	2147.037	-56.074
2100	1074.797	2135.981	1372.359	1603.607	561.288	2226.398	-55.377
2200	1081.161	2186.131	1408.217	1711.411	564.208	2305.621	-54.741
2300	1086.828	2234.318	1443.093	1819.816	566.977	2384.712	-54.157
2400	1091.894	2280.682	1477.033	1928.757	569.519	2463.636	-53.619
2500	1096.438	2325.349	1510.078	2038.177	571.845	2542.580	-53.123
2600	1100.526	2368.433	1542.268	2148.029	573.914	2621.311	-52.662
2700	1104.217	2410.038	1573.641	2258.269	575.733	2700.043	-52.234
2800	1107.558	2450.257	1604.235	2368.861	577.271	2778.738	-51.837
2900	1110.592	2489.176	1634.083	2479.771	578.497	2857.325	-51.465
3000	1113.354	2526.874	1663.217	2590.970	579.457	2935.903	-51.118
3100	1115.875	2563.423	1691.670	2702.433	580.069	3014.373	-50.791
3200	1118.182	2598.887	1719.469	2814.138	580.375	3092.906	-50.485
3300	1120.298	2633.328	1746.642	2926.063	580.357	3171.476	-50.199
3400	1122.242	2666.802	1773.216	3038.192	579.984	3249.961	-49.929
3500	1124.034	2699.359	1799.214	3150.507	579.261	3328.441	-49.673
3600	1125.688	2731.048	1824.660	3262.994	578.211	3407.039	-49.434
3700	1127.217	2761.911	1849.576	3375.640	576.802	3485.692	-49.208
3800	1128.634	2791.991	1873.982	3488.434	575.002	3564.320	-48.994
3900	1129.949	2821.325	1897.899	3601.364	572.858	3642.948	-48.791
4000	1131.172	2849.949	1921.344	3714.420	570.351	3721.784	-48.601
4100	1132.311	2877.894	1944.335	3827.595	567.442	3800.606	-48.419
4200	1133.373	2905.193	1966.889	3940.880	564.163	3879.495	-48.248
4300	1134.366	2931.874	1989.021	4054.267	560.497	3958.370	-48.084
4400	1135.294	2957.963	2010.747	4167.751	556.454	4037.434	-47.929
4500	1136.164	2983.486	2032.081	4281.324	552.050	4116.656	-47.784
4600	1136.979	3008.467	2053.036	4394.982	547.228	4195.985	-47.646
4700	1137.746	3032.927	2073.626	4508.719	542.005	4275.302	-47.514
4800	1138.466	3056.888	2093.861	4622.529	536.431	4354.848	-47.389
4900	1139.145	3080.370	2113.755	4736.410	530.426	4434.369	-47.270
5000	1139.784	3103.390	2133.319	4850.357	524.091	4514.220	-47.159

3.375. 4*H*-Dibenzo[*a,de*]pentacene



Formula: C₂₉H₁₈
Mass: 366.453 g/mol
CAS Number: 198-45-8
Point Group: C_s

Length: 18.34 Å
Width: 11.05 Å
Breadth: 4.171 Å
L/B Ratio: 1.659

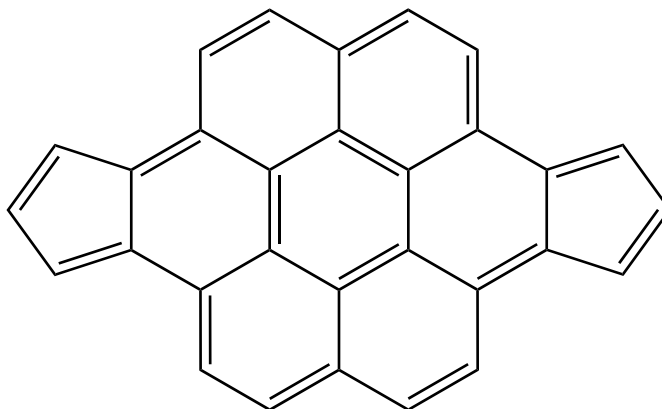
Cartesian coordinates:

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C	-6.0736	-1.8256	0.0000	C	1.0027	2.9925	0.0000	H	-3.9330	2.2693	0.0000
C	-6.3023	0.9755	0.0000	C	3.4987	1.7481	0.0000	H	-1.0795	-2.5145	0.0000
C	-4.9916	0.3881	0.0000	C	2.3335	0.9600	0.0000	H	-1.4812	2.4723	0.0000
C	-4.8755	-1.0333	0.0000	C	2.4141	-0.4905	0.0000	H	1.3419	-2.3357	0.0000
C	-3.6175	-1.6247	0.0000	C	4.8598	1.1416	0.0000	H	4.3132	3.7442	0.0000
C	-3.8461	1.1758	0.0000	C	4.8993	-0.3470	0.0000	H	2.0898	4.8497	0.0000
C	-2.5723	0.5834	0.0000	C	3.7352	-1.1243	0.0000	H	0.0120	3.4725	0.0000
C	-2.4564	-0.8336	0.0000	C	3.8527	-2.5213	0.0000	H	5.4166	1.5134	-0.8861
C	-1.1634	-1.4205	0.0000	C	5.0972	-3.1315	0.0000	H	5.4166	1.5134	0.8861
C	-1.3926	1.3738	0.0000	C	6.2520	-2.3536	0.0000	H	2.9374	-3.1329	0.0000
C	-0.1449	0.7928	0.0000	C	6.1511	-0.9702	0.0000	H	5.1715	-4.2238	0.0000
C	-0.0317	-0.6354	0.0000	H	-8.4121	0.6347	0.0000	H	7.2366	-2.8322	0.0000
C	1.2791	-1.2351	0.0000	H	-8.2107	-1.8316	0.0000	H	7.0583	-0.3552	0.0000
C	1.0742	1.5907	0.0000	H	-5.9746	-2.9170	0.0000				

Table 3.375: Table of thermodynamic data as a function of temperature for 4*H*-Dibenzo[*a,de*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.741	479.486	479.486	∞
100	123.758	375.431	856.065	-48.063	509.373	565.245	-295.248
200	240.334	495.066	645.760	-30.139	493.598	627.402	-163.857
250	308.153	555.920	621.680	-16.440	486.149	661.715	-138.255
298.15	374.600	615.887	615.887	0.000	479.486	696.149	-121.960
300	377.128	618.212	615.894	0.695	479.240	697.492	-121.442
350	443.744	681.397	620.732	21.233	473.077	734.369	-109.596
400	505.737	744.757	632.277	44.992	467.716	772.061	-100.819
450	562.055	807.634	648.275	71.711	463.074	810.388	-94.065
500	612.519	869.515	667.315	101.100	459.062	849.221	-88.716
600	697.413	988.996	711.059	166.762	452.602	927.894	-80.779
700	764.818	1101.759	758.902	240.000	447.981	1007.506	-75.179
800	819.068	1207.554	808.443	319.289	444.983	1087.649	-71.015
900	863.404	1306.671	858.355	403.484	443.398	1168.075	-67.792
1000	900.113	1399.598	907.882	491.716	443.027	1248.625	-65.220
1100	930.818	1486.871	956.592	583.307	443.641	1329.173	-63.116
1200	956.711	1569.004	1004.238	677.719	445.072	1409.608	-61.357
1300	978.698	1646.473	1050.689	774.519	447.112	1489.910	-59.864
1400	997.481	1719.708	1095.885	873.352	449.609	1570.042	-58.578
1500	1013.616	1789.091	1139.806	973.927	452.466	1649.983	-57.456
1600	1027.551	1854.964	1182.463	1076.002	455.537	1729.716	-56.468
1700	1039.644	1917.630	1223.880	1179.376	458.737	1809.226	-55.590
1800	1050.190	1977.360	1264.094	1283.880	461.981	1888.616	-54.805
1900	1059.429	2034.394	1303.146	1389.371	465.233	1967.769	-54.097
2000	1067.558	2088.946	1341.082	1495.728	468.430	2046.779	-53.455
2100	1074.740	2141.210	1377.948	1602.851	471.487	2125.617	-52.871
2200	1081.111	2191.357	1413.789	1710.649	474.402	2204.317	-52.336
2300	1086.785	2239.542	1448.651	1819.050	477.166	2282.885	-51.845
2400	1091.856	2285.904	1482.577	1927.986	479.704	2361.287	-51.391
2500	1096.404	2330.570	1515.608	2037.403	482.026	2439.709	-50.974
2600	1100.497	2373.653	1547.786	2147.252	484.093	2517.918	-50.585
2700	1104.190	2415.256	1579.149	2257.489	485.908	2596.128	-50.224
2800	1107.535	2455.474	1609.732	2368.078	487.444	2674.302	-49.889
2900	1110.571	2494.393	1639.570	2478.986	488.668	2752.367	-49.574
3000	1113.335	2532.090	1668.696	2590.184	489.626	2830.423	-49.281
3100	1115.858	2568.638	1697.140	2701.645	490.236	2908.371	-49.005
3200	1118.167	2604.102	1724.931	2813.348	490.541	2986.383	-48.747
3300	1120.284	2638.543	1752.097	2925.272	490.521	3064.432	-48.505
3400	1122.230	2672.016	1778.663	3037.399	490.147	3142.395	-48.276
3500	1124.022	2704.573	1804.655	3149.713	489.423	3220.354	-48.060
3600	1125.677	2736.261	1830.095	3262.199	488.372	3298.430	-47.858
3700	1127.207	2767.125	1855.005	3374.844	486.961	3376.562	-47.668
3800	1128.625	2797.204	1879.405	3487.637	485.160	3454.669	-47.487
3900	1129.941	2826.538	1903.316	3600.566	483.015	3532.776	-47.315
4000	1131.164	2855.161	1926.756	3713.622	480.507	3611.090	-47.155
4100	1132.304	2883.107	1949.742	3826.796	477.598	3689.391	-47.002
4200	1133.366	2910.406	1972.291	3940.080	474.319	3767.758	-46.858
4300	1134.359	2937.086	1994.419	4053.467	470.651	3846.112	-46.720
4400	1135.288	2963.175	2016.141	4166.950	466.608	3924.655	-46.591
4500	1136.158	2988.698	2037.471	4280.522	462.203	4003.355	-46.469
4600	1136.974	3013.679	2058.422	4394.179	457.381	4082.164	-46.353
4700	1137.741	3038.139	2079.008	4507.915	452.157	4160.960	-46.243
4800	1138.462	3062.100	2099.240	4621.726	446.583	4239.984	-46.139
4900	1139.141	3085.581	2119.131	4735.606	440.577	4318.984	-46.040
5000	1139.780	3108.602	2138.691	4849.553	434.242	4398.314	-45.948

3.376. Dicyclopenta[*a,j*]coronene



Formula: C₃₀H₁₄
Mass: 374.432 g/mol
CAS Number: 90207-46-8
Point Group: D_{2h}

Length: 16.25 Å
Width: 11.68 Å
Breadth: 3.890 Å
L/B Ratio: 1.392

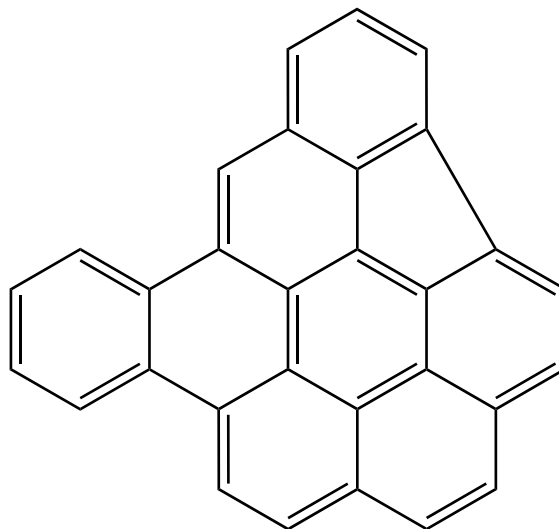
Cartesian coordinates:

C	4.9747	-1.2059	-0.0002	C	-3.6727	0.7836	-0.0005	H	6.9256	-0.0790	0.0000
C	3.6728	-0.7836	-0.0001	C	-2.4251	1.5028	-0.0007	H	5.3426	-2.2300	-0.0004
C	3.6645	0.6866	0.0002	C	-4.9747	1.2059	-0.0008	H	5.4044	2.1340	0.0004
C	5.0701	1.0986	0.0003	C	-5.8390	0.0256	-0.0005	H	1.3136	4.6264	0.0007
C	5.8390	-0.0256	0.0000	C	-5.0701	-1.0986	0.0019	H	3.4506	3.3693	0.0008
C	2.5082	1.3999	0.0002	C	0.0494	2.8438	0.0001	H	-3.2974	3.4656	-0.0008
C	1.2398	0.6824	0.0000	C	-1.1320	3.5505	-0.0001	H	-1.1209	4.6469	0.0002
C	1.2136	-0.7297	-0.0001	C	-2.3711	2.8789	-0.0006	H	-1.3136	-4.6264	-0.0007
C	2.4251	-1.5028	-0.0002	C	-0.0495	-2.8438	-0.0002	H	-3.4506	-3.3693	-0.0001
C	0.0334	1.4099	-0.0001	C	-1.3256	-3.5299	-0.0002	H	3.2974	-3.4656	-0.0004
C	-1.2136	0.7297	-0.0004	C	-2.4854	-2.8484	0.0001	H	1.1209	-4.6469	-0.0005
C	-1.2398	-0.6824	-0.0000	C	2.3711	-2.8789	-0.0003	H	-5.4044	-2.1340	0.0020
C	-0.0334	-1.4099	-0.0001	C	1.1320	-3.5505	-0.0003	H	-6.9255	0.0790	0.0006
C	-2.5082	-1.3999	0.0005	C	2.4854	2.8484	0.0005	H	-5.3426	2.2300	-0.0017
C	-3.6645	-0.6866	0.0010	C	1.3256	3.5300	0.0005				

Table 3.376: Table of thermodynamic data as a function of temperature for Dicyclopenta[*a,j*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-52.382	721.433	721.433	∞
100	110.898	336.235	794.372	-45.814	743.626	783.367	-409.181
200	229.514	447.717	592.983	-29.053	731.748	827.874	-216.214
250	297.231	506.164	569.740	-15.894	726.255	852.539	-178.125
298.15	362.712	564.136	564.136	0.000	721.433	877.313	-153.699
300	365.189	566.387	564.143	0.673	721.256	878.278	-152.919
350	430.097	627.610	568.830	20.573	716.883	904.806	-135.032
400	489.974	689.013	580.017	43.599	713.149	931.904	-121.692
450	543.976	749.901	595.518	69.472	709.956	959.445	-111.367
500	592.046	809.753	613.959	97.897	707.206	987.339	-103.145
600	672.149	925.077	656.291	161.272	702.738	1043.809	-90.870
700	734.920	1033.595	702.524	231.750	699.460	1100.936	-82.151
800	784.792	1135.108	750.324	307.827	697.237	1158.443	-75.637
900	825.074	1229.951	798.407	388.390	695.931	1216.164	-70.583
1000	858.087	1318.645	846.045	472.601	695.424	1274.001	-66.546
1100	885.470	1401.753	892.826	559.820	695.550	1331.868	-63.244
1200	908.404	1479.811	938.523	649.547	696.201	1389.679	-60.490
1300	927.771	1553.309	983.015	741.382	697.219	1447.433	-58.157
1400	944.241	1622.683	1026.251	835.004	698.494	1505.101	-56.155
1500	958.340	1688.322	1068.221	930.151	699.965	1562.675	-54.416
1600	970.479	1750.569	1108.939	1026.607	701.514	1620.137	-52.891
1700	980.989	1809.726	1148.436	1124.193	703.081	1677.476	-51.542
1800	990.136	1866.063	1186.752	1222.760	704.600	1734.792	-50.341
1900	998.136	1919.816	1223.931	1322.182	706.048	1791.969	-49.264
2000	1005.164	1971.196	1260.019	1422.354	707.381	1849.100	-48.293
2100	1011.367	2020.392	1295.064	1523.187	708.522	1906.155	-47.412
2200	1016.864	2067.570	1329.113	1624.604	709.476	1963.159	-46.610
2300	1021.754	2112.881	1362.212	1726.540	710.244	2020.129	-45.878
2400	1026.122	2156.461	1394.403	1828.938	710.755	2077.014	-45.204
2500	1030.036	2198.430	1425.730	1931.749	711.027	2134.005	-44.587
2600	1033.557	2238.898	1456.232	2034.932	711.023	2190.865	-44.014
2700	1036.732	2277.966	1485.947	2138.449	710.752	2247.812	-43.486
2800	1039.606	2315.722	1514.912	2242.268	710.189	2304.792	-42.996
2900	1042.214	2352.249	1543.159	2346.361	709.304	2361.743	-42.539
3000	1044.588	2387.623	1570.721	2450.703	708.147	2418.760	-42.113
3100	1046.754	2421.910	1597.629	2555.272	706.636	2475.733	-41.715
3200	1048.735	2455.175	1623.910	2660.048	704.817	2532.843	-41.344
3300	1050.551	2487.475	1649.592	2765.014	702.675	2590.058	-40.996
3400	1052.220	2518.862	1674.699	2870.153	700.177	2647.245	-40.669
3500	1053.757	2549.386	1699.256	2975.453	697.332	2704.492	-40.362
3600	1055.176	2579.091	1723.285	3080.901	694.164	2761.925	-40.074
3700	1056.488	2608.020	1746.808	3186.485	690.640	2819.462	-39.803
3800	1057.703	2636.211	1769.844	3292.195	686.736	2877.041	-39.547
3900	1058.830	2663.700	1792.412	3398.023	682.492	2934.664	-39.305
4000	1059.879	2690.521	1814.531	3503.959	677.894	2992.556	-39.078
4100	1060.855	2716.704	1836.217	3609.996	672.904	3050.486	-38.863
4200	1061.765	2742.279	1857.487	3716.127	667.553	3108.534	-38.659
4300	1062.615	2767.273	1878.355	3822.347	661.826	3166.615	-38.466
4400	1063.411	2791.711	1898.836	3928.649	655.733	3224.932	-38.284
4500	1064.156	2815.617	1918.945	4035.027	649.291	3283.449	-38.112
4600	1064.855	2839.014	1938.693	4141.478	642.442	3342.130	-37.950
4700	1065.511	2861.922	1958.093	4247.997	635.204	3400.838	-37.795
4800	1066.128	2884.361	1977.157	4354.579	627.626	3459.820	-37.650
4900	1066.709	2906.350	1995.897	4461.221	619.628	3518.814	-37.510
5000	1067.257	2927.906	2014.322	4567.920	611.311	3578.175	-37.380

3.377. Dibenz[*e,ghi*]indeno[1,2,3,4-*pqra*]perylene



Formula: C₃₀H₁₄
Mass: 374.432 g/mol
CAS Number: 75449-96-6
Point Group: C₁

Length: 13.77 Å
Width: 12.34 Å
Breadth: 4.630 Å
L/B Ratio: 1.115

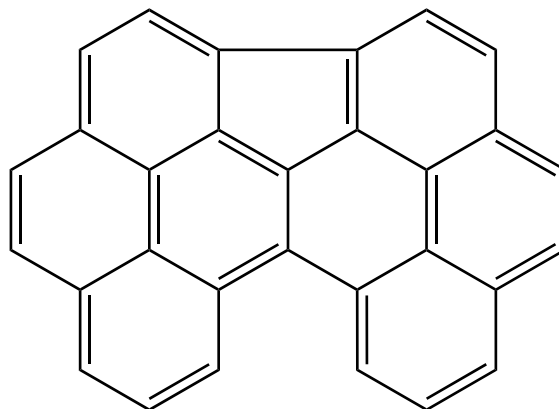
Cartesian coordinates:

C	-4.4601	-0.7052	0.0951	C	4.0286	-1.7693	0.1759	H	-1.6238	3.5798	0.1159
C	-3.1094	-0.3430	-0.0101	C	4.2314	-0.3777	0.1178	H	-3.4033	-3.0825	0.2254
C	-2.7736	1.0349	-0.0425	C	3.1553	0.4721	-0.1405	H	-1.5670	-4.7628	0.3122
C	-3.7921	1.9929	0.0420	C	1.3716	2.0075	-0.2678	H	0.9248	-5.2751	0.3308
C	-5.1190	1.6105	0.1419	C	2.8040	1.9292	-0.0778	H	3.2639	-4.4864	0.3632
C	-5.4536	0.2563	0.1656	C	0.5039	3.0708	-0.0440	H	4.8946	-2.4117	0.3737
C	-1.3815	1.4638	-0.1594	C	-0.8977	2.7678	-0.0360	H	5.2318	0.0270	0.3004
C	-0.4647	0.3921	-0.3518	C	0.0221	-3.3167	0.0416	H	4.4725	3.2066	0.4183
C	-0.7653	-1.0103	-0.2422	C	-1.3298	-3.7038	0.1596	H	3.0766	5.2250	0.5912
C	-2.0920	-1.3961	-0.0589	C	-2.3532	-2.7713	0.1123	H	0.6252	5.2083	0.4008
C	0.2942	-1.9615	-0.1894	C	2.4410	-3.7792	0.2122	H	-3.5092	3.0561	0.0299
C	1.6695	-1.5476	-0.2313	C	1.1487	-4.2100	0.1983	H	-5.9057	2.3693	0.2031
C	1.9370	-0.1991	-0.3787	C	1.1957	4.2859	0.2517	H	-6.5032	-0.0456	0.2420
C	0.8553	0.7218	-0.4642	C	2.5675	4.2810	0.3635	H	-4.7099	-1.7777	0.1244
C	2.7667	-2.3843	0.0407	C	3.3971	3.1185	0.2379				

Table 3.377: Table of thermodynamic data as a function of temperature for Dibenz[*e,ghi*]indeno[1,2,3,4-*pqra*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-50.786	571.408	571.408	∞
100	105.629	348.017	791.481	-44.346	595.067	633.631	-330.968
200	222.025	455.025	596.242	-28.243	582.533	677.196	-176.862
250	288.928	511.711	573.629	-15.479	576.644	701.542	-146.576
298.15	353.842	568.168	568.168	0.000	571.408	726.086	-127.205
300	356.302	570.364	568.175	0.657	571.214	727.043	-126.587
350	420.948	630.194	572.752	20.105	566.388	753.408	-112.438
400	480.854	690.374	583.694	42.672	562.197	780.408	-101.909
450	535.108	750.200	598.877	68.095	558.553	807.908	-93.778
500	583.581	809.138	616.965	96.086	555.370	835.811	-87.315
600	664.720	923.007	658.566	158.665	550.106	892.419	-77.690
700	728.589	1030.463	704.099	228.455	546.140	949.808	-70.874
800	779.470	1131.198	751.259	303.951	543.335	1007.669	-65.793
900	820.619	1225.465	798.770	384.026	541.542	1065.811	-61.857
1000	854.355	1313.729	845.900	467.829	540.626	1124.119	-58.717
1100	882.328	1396.510	892.233	554.705	540.410	1182.495	-56.151
1200	905.743	1474.316	937.531	644.142	540.771	1240.844	-54.011
1300	925.500	1547.616	981.668	735.732	541.544	1299.158	-52.200
1400	942.290	1616.834	1024.588	829.144	542.608	1357.403	-50.644
1500	956.650	1682.348	1066.275	924.109	543.897	1415.569	-49.293
1600	969.005	1744.493	1106.738	1020.407	545.288	1473.633	-48.108
1700	979.694	1803.567	1146.005	1117.855	546.718	1531.584	-47.059
1800	988.991	1859.834	1184.112	1216.300	548.114	1589.520	-46.126
1900	997.117	1913.528	1221.100	1315.614	549.455	1647.322	-45.287
2000	1004.253	1964.859	1257.014	1415.690	550.691	1705.085	-44.531
2100	1010.547	2014.012	1291.899	1516.436	551.745	1762.775	-43.846
2200	1016.123	2061.154	1325.801	1617.775	552.621	1820.420	-43.221
2300	1021.082	2106.434	1358.764	1719.640	553.319	1878.032	-42.651
2400	1025.509	2149.986	1390.830	1821.974	553.766	1935.564	-42.126
2500	1029.475	2191.931	1422.040	1924.727	553.979	1993.203	-41.645
2600	1033.041	2232.379	1452.434	2027.856	553.922	2050.714	-41.199
2700	1036.257	2271.427	1482.048	2131.323	553.601	2108.315	-40.787
2800	1039.167	2309.167	1510.918	2235.097	552.992	2165.949	-40.405
2900	1041.807	2345.679	1539.077	2339.148	552.065	2223.557	-40.050
3000	1044.209	2381.039	1566.556	2443.450	550.868	2281.231	-39.719
3100	1046.400	2415.315	1593.385	2547.982	549.320	2338.863	-39.409
3200	1048.404	2448.569	1619.593	2652.724	547.468	2396.633	-39.120
3300	1050.242	2480.859	1645.205	2757.658	545.294	2454.509	-38.851
3400	1051.930	2512.237	1670.247	2862.768	542.765	2512.358	-38.597
3500	1053.484	2542.753	1694.741	2968.039	539.892	2570.268	-38.358
3600	1054.919	2572.451	1718.712	3073.460	536.698	2628.365	-38.136
3700	1056.245	2601.373	1742.178	3179.019	533.149	2686.566	-37.927
3800	1057.473	2629.557	1765.161	3284.706	529.221	2744.810	-37.729
3900	1058.613	2657.041	1787.679	3390.511	524.955	2803.099	-37.543
4000	1059.673	2683.856	1809.749	3496.426	520.336	2861.657	-37.369
4100	1060.659	2710.034	1831.390	3602.443	515.326	2920.254	-37.204
4200	1061.579	2735.605	1852.615	3708.556	509.956	2978.969	-37.048
4300	1062.438	2760.594	1873.442	3814.757	504.211	3037.718	-36.900
4400	1063.242	2785.029	1893.883	3921.041	498.100	3096.703	-36.762
4500	1063.995	2808.931	1913.953	4027.404	491.642	3155.888	-36.632
4600	1064.701	2832.324	1933.664	4133.839	484.777	3215.238	-36.509
4700	1065.364	2855.229	1953.029	4240.342	477.524	3274.615	-36.393
4800	1065.987	2877.665	1972.059	4346.910	469.931	3334.267	-36.283
4900	1066.574	2899.651	1990.766	4453.539	461.920	3393.930	-36.179
5000	1067.127	2921.205	2009.160	4560.224	453.590	3453.961	-36.083

3.378. Dibenzo[*mn,qr*]fluoreno[2,1,9,8,7-*defghi*]naphthacene



Formula: C₃₀H₁₄
Mass: 374.432 g/mol
CAS Number: 76759-99-4
Point Group: C_{2v}

Length: 14.29 Å
Width: 11.51 Å
Breadth: 3.885 Å
L/B Ratio: 1.241

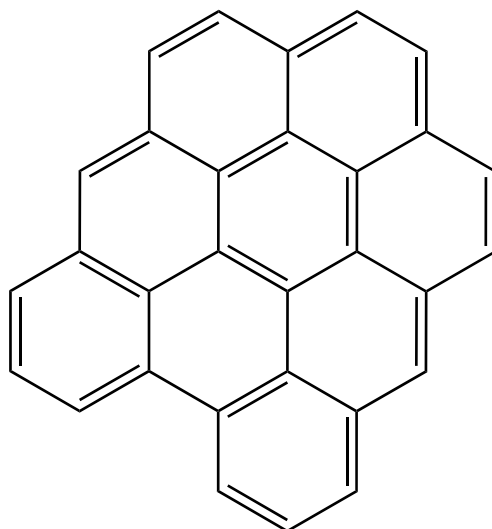
Cartesian coordinates:

C	-0.7586	2.5641	0.0000	C	-1.3507	-1.6251	0.0000	H	-3.9680	3.6852	0.0000
C	-1.1273	1.1956	0.0000	C	-2.3960	0.6691	0.0000	H	-1.6512	4.5371	0.0000
C	-0.0016	0.3227	0.0000	C	0.0052	-1.0427	0.0000	H	-5.6457	1.6856	0.0000
C	1.1154	1.2067	0.0000	C	3.1138	2.9940	0.0000	H	-5.9400	-0.7695	0.0000
C	0.7332	2.5715	0.0000	C	1.7889	3.4742	0.0000	H	-5.0346	-3.0567	0.0000
C	-3.1433	2.9630	0.0000	C	1.3668	-1.6115	0.0000	H	-3.0751	-4.5759	0.0000
C	-1.8232	3.4563	0.0000	C	1.6469	-2.9785	0.0000	H	-0.8003	-3.7253	0.0000
C	-3.4606	1.5950	0.0000	C	2.9542	-3.4622	0.0000	H	3.9313	3.7244	0.0000
C	-4.7796	1.0152	0.0000	C	4.0445	-2.6066	0.0000	H	1.6062	4.5532	0.0000
C	-4.9337	-0.3333	0.0000	C	2.3893	0.6928	0.0000	H	0.8370	-3.7169	0.0000
C	-3.8212	-1.2615	0.0000	C	2.5094	-0.7370	0.0000	H	3.1203	-4.5452	0.0000
C	-4.0185	-2.6466	0.0000	C	3.8335	-1.2235	0.0000	H	5.0646	-3.0066	0.0000
C	-2.9198	-3.4913	0.0000	C	4.9367	-0.2843	0.0000	H	5.9473	-0.7106	0.0000
C	-1.6173	-2.9947	0.0000	C	4.7693	1.0625	0.0000	H	5.6287	1.7415	0.0000
C	-2.5020	-0.7619	0.0000	C	3.4447	1.6293	0.0000				

Table 3.378: Table of thermodynamic data as a function of temperature for Dibenzo[*mn,qr*]fluoreno[2,1,9,8,7-*defghi*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-50.789	561.627	561.627	∞
100	105.202	341.394	785.168	-44.377	585.255	624.481	-326.189
200	222.294	448.298	589.722	-28.285	572.710	668.719	-174.648
250	289.376	505.066	567.076	-15.502	566.840	693.399	-144.875
298.15	354.330	561.607	561.607	0.000	561.627	718.261	-125.834
300	356.790	563.806	561.614	0.658	561.434	719.230	-125.227
350	421.418	623.710	566.197	20.130	556.632	745.921	-111.320
400	481.288	683.951	577.152	42.720	552.463	773.244	-100.973
450	535.502	743.825	592.351	68.164	548.840	801.064	-92.983
500	583.936	802.803	610.456	96.173	545.676	829.284	-86.633
600	665.000	916.730	652.091	158.784	540.443	886.522	-77.177
700	728.799	1024.224	697.655	228.598	536.502	944.538	-70.481
800	779.618	1124.983	744.843	304.112	533.715	1003.021	-65.489
900	820.716	1219.264	792.377	384.199	531.934	1061.784	-61.623
1000	854.411	1307.536	839.527	468.009	531.026	1120.712	-58.539
1100	882.353	1390.321	885.876	554.890	530.813	1179.707	-56.018
1200	905.745	1468.128	931.188	644.328	531.176	1238.675	-53.917
1300	925.485	1541.427	975.337	735.917	531.948	1297.607	-52.137
1400	942.263	1610.644	1018.267	829.327	533.010	1356.472	-50.610
1500	956.615	1676.155	1059.963	924.289	534.296	1415.256	-49.283
1600	968.965	1738.298	1100.433	1020.583	535.683	1473.939	-48.118
1700	979.651	1797.369	1139.707	1118.027	537.108	1532.511	-47.087
1800	988.946	1853.634	1177.819	1216.467	538.501	1591.066	-46.171
1900	997.071	1907.326	1214.812	1315.777	539.837	1649.488	-45.347
2000	1004.207	1958.654	1250.730	1415.848	541.068	1707.872	-44.604
2100	1010.502	2007.805	1285.619	1516.590	542.118	1766.183	-43.930
2200	1016.079	2054.945	1319.525	1617.925	542.990	1824.448	-43.317
2300	1021.039	2100.223	1352.490	1719.786	543.683	1882.681	-42.756
2400	1025.467	2143.773	1384.559	1822.115	544.126	1940.834	-42.240
2500	1029.435	2185.717	1415.771	1924.864	544.334	1999.095	-41.768
2600	1033.002	2226.163	1446.167	2027.989	544.273	2057.227	-41.329
2700	1036.220	2265.210	1475.783	2131.452	543.949	2115.449	-40.925
2800	1039.131	2302.948	1504.655	2235.222	543.336	2173.705	-40.550
2900	1041.773	2339.460	1532.815	2339.270	542.405	2231.935	-40.201
3000	1044.176	2374.818	1560.295	2443.569	541.206	2290.231	-39.876
3100	1046.369	2409.093	1587.126	2548.098	539.655	2348.486	-39.571
3200	1048.375	2442.346	1613.335	2652.837	537.799	2406.877	-39.287
3300	1050.213	2474.635	1638.948	2757.767	535.622	2465.377	-39.023
3400	1051.902	2506.012	1663.990	2862.874	533.091	2523.848	-38.773
3500	1053.458	2536.527	1688.486	2968.143	530.215	2582.380	-38.539
3600	1054.893	2566.224	1712.457	3073.562	527.019	2641.099	-38.321
3700	1056.221	2595.146	1735.924	3179.118	523.467	2699.923	-38.115
3800	1057.450	2623.330	1758.908	3284.803	519.536	2758.790	-37.921
3900	1058.591	2650.812	1781.426	3390.605	515.268	2817.702	-37.738
4000	1059.651	2677.627	1803.498	3496.518	510.647	2876.882	-37.567
4100	1060.639	2703.805	1825.138	3602.533	505.635	2936.103	-37.406
4200	1061.559	2729.375	1846.365	3708.644	500.262	2995.440	-37.253
4300	1062.419	2754.364	1867.191	3814.843	494.516	3054.812	-37.108
4400	1063.224	2778.798	1887.633	3921.126	488.403	3114.420	-36.972
4500	1063.977	2802.700	1907.703	4027.486	481.943	3174.229	-36.845
4600	1064.684	2826.093	1927.415	4133.920	475.076	3234.202	-36.725
4700	1065.347	2848.998	1946.780	4240.421	467.822	3294.202	-36.610
4800	1065.971	2871.433	1965.811	4346.988	460.227	3354.477	-36.503
4900	1066.559	2893.419	1984.518	4453.615	452.214	3414.764	-36.401
5000	1067.113	2914.972	2002.912	4560.298	443.883	3475.418	-36.307

3.379. Dibenzo[bc,ef]coronene



Other names: Anthrodianthrene
2,3,4,5-Dibenzocoronene
vic-diperi-Dibenzocoronene

Formula: C₃₀H₁₄
Mass: 374.432 g/mol
CAS Number: 190-31-8
Point Group: C_{2v}

Length: 12.85 Å
Width: 11.68 Å
Breadth: 3.885 Å
L/B Ratio: 1.100

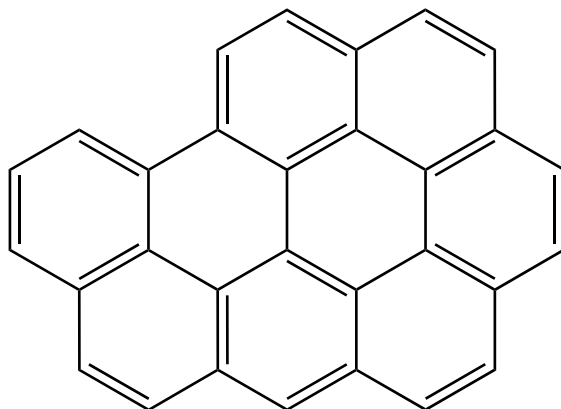
Cartesian coordinates:

C	-3.9917	-1.4080	0.0000	C	-1.5688	-1.4114	0.0000	H	-4.9460	-0.8588	0.0000
C	-3.9915	-2.8178	0.0000	C	-2.7916	0.7606	0.0000	H	-4.9500	-3.3473	0.0000
C	-2.8130	-3.5156	0.0000	C	-2.7367	3.5753	0.0000	H	-2.8101	-4.6114	0.0000
C	-1.5706	-2.8253	0.0000	C	-3.9299	2.9030	0.0000	H	-0.3617	-4.6286	0.0000
C	-0.3444	-3.5317	0.0000	C	-3.9605	1.4936	0.0000	H	2.1009	-4.6512	0.0000
C	0.8605	-2.8556	0.0000	C	-1.5094	2.8585	0.0000	H	4.2544	-3.4238	0.0000
C	2.1249	-3.5553	0.0000	C	-1.5380	1.4449	0.0000	H	5.4953	-1.2991	0.0000
C	3.2990	-2.8864	0.0000	C	-0.3156	0.7237	0.0000	H	5.5220	1.1805	0.0000
C	3.3375	-1.4444	0.0000	C	-0.2683	3.5383	0.0000	H	-2.7102	4.6709	0.0000
C	4.5522	-0.7406	0.0000	C	0.9218	2.8364	0.0000	H	-4.8769	3.4530	0.0000
C	4.5671	0.6424	0.0000	C	0.9028	1.4098	0.0000	H	-4.9264	0.9651	0.0000
C	2.1246	-0.7306	0.0000	C	2.1398	0.6847	0.0000	H	-0.2619	4.6353	0.0000
C	0.8723	-1.4289	0.0000	C	3.3679	1.3721	0.0000	H	4.3271	3.3314	0.0000
C	-0.3311	-0.7167	0.0000	C	3.3604	2.8147	0.0000	H	2.2006	4.6049	0.0000
C	-2.8074	-0.7004	0.0000	C	2.2009	3.5087	0.0000				

Table 3.379: Table of thermodynamic data as a function of temperature for Dibenzo[bc,ef]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-49.924	437.665	437.665	∞
100	101.102	332.594	771.308	-43.871	461.800	501.905	-262.163
200	220.035	437.346	577.737	-28.078	448.955	547.154	-142.899
250	287.301	493.636	555.247	-15.403	442.978	572.394	-119.593
298.15	352.259	549.812	549.812	0.000	437.665	597.816	-104.733
300	354.719	551.999	549.819	0.654	437.468	598.807	-104.259
350	419.335	611.582	554.377	20.022	432.563	626.096	-93.438
400	479.239	671.546	565.275	42.508	428.290	654.033	-85.406
450	533.539	731.184	580.402	67.852	424.567	682.479	-79.218
500	582.096	789.961	598.428	95.766	421.307	711.336	-74.311
600	663.455	903.579	639.900	158.207	415.905	769.875	-67.022
700	727.546	1010.856	685.310	227.882	411.824	829.217	-61.876
800	778.618	1111.465	732.360	303.284	408.925	889.045	-58.048
900	819.921	1205.641	779.773	383.281	407.054	949.166	-55.087
1000	853.780	1293.838	826.817	467.020	406.075	1009.460	-52.728
1100	881.850	1376.569	873.073	553.845	405.807	1069.828	-50.801
1200	905.341	1454.336	918.305	643.238	406.124	1130.173	-49.194
1300	925.159	1527.607	962.383	734.791	406.860	1190.486	-47.833
1400	941.998	1596.801	1005.251	828.171	407.892	1250.733	-46.664
1500	956.397	1662.296	1046.890	923.109	409.154	1310.903	-45.649
1600	968.785	1724.426	1087.311	1019.383	410.521	1370.973	-44.757
1700	979.501	1783.487	1126.540	1116.810	411.930	1430.932	-43.966
1800	988.820	1839.744	1164.612	1215.237	413.309	1490.876	-43.263
1900	996.965	1893.430	1201.569	1314.535	414.633	1550.687	-42.630
2000	1004.116	1944.753	1237.455	1414.597	415.855	1610.461	-42.060
2100	1010.424	1993.900	1272.314	1515.330	416.896	1670.162	-41.542
2200	1016.012	2041.036	1306.192	1616.658	417.761	1729.818	-41.070
2300	1020.980	2086.312	1339.132	1718.512	418.448	1789.442	-40.639
2400	1025.416	2129.860	1371.178	1820.836	418.885	1848.986	-40.241
2500	1029.390	2171.801	1402.369	1923.580	419.089	1908.639	-39.878
2600	1032.963	2212.245	1432.745	2026.701	419.024	1968.162	-39.540
2700	1036.185	2251.291	1462.343	2130.161	418.696	2027.776	-39.229
2800	1039.100	2289.028	1491.197	2233.927	418.079	2087.424	-38.941
2900	1041.745	2325.539	1519.341	2337.972	417.146	2147.046	-38.672
3000	1044.151	2360.897	1546.807	2442.268	415.943	2206.735	-38.422
3100	1046.346	2395.170	1573.624	2546.795	414.390	2266.381	-38.187
3200	1048.354	2428.423	1599.819	2651.531	412.532	2326.165	-37.970
3300	1050.195	2460.711	1625.420	2756.460	410.353	2386.057	-37.767
3400	1051.886	2492.088	1650.451	2861.565	407.820	2445.921	-37.576
3500	1053.443	2522.602	1674.936	2966.833	404.943	2505.845	-37.397
3600	1054.879	2552.299	1698.896	3072.250	401.745	2565.957	-37.230
3700	1056.208	2581.220	1722.354	3177.805	398.192	2626.173	-37.074
3800	1057.438	2609.404	1745.328	3283.488	394.260	2686.433	-36.927
3900	1058.580	2636.886	1767.837	3389.290	389.991	2746.737	-36.788
4000	1059.641	2663.700	1789.900	3495.201	385.368	2807.310	-36.659
4100	1060.629	2689.878	1811.533	3601.215	380.355	2867.923	-36.537
4200	1061.550	2715.448	1832.751	3707.325	374.982	2928.654	-36.422
4300	1062.411	2740.437	1853.571	3813.523	369.234	2989.419	-36.313
4400	1063.216	2764.870	1874.006	3919.805	363.121	3050.419	-36.212
4500	1063.970	2788.773	1894.069	4026.165	356.660	3111.621	-36.118
4600	1064.677	2812.165	1913.774	4132.598	349.793	3172.986	-36.030
4700	1065.341	2835.070	1933.134	4239.099	342.538	3234.379	-35.945
4800	1065.965	2857.505	1952.158	4345.665	334.943	3296.047	-35.868
4900	1066.553	2879.491	1970.860	4452.291	326.929	3357.727	-35.793
5000	1067.107	2901.044	1989.249	4558.974	318.597	3419.774	-35.725

3.380. Naphtho[8,1,2-*abc*]coronene



Other names: Naphtho[5,4,3-*abc*]coronene

Formula: C₃₀H₁₄

Mass: 374.432 g/mol

CAS Number: 6596-38-9

Point Group: C_s

Length: 14.09 Å

Width: 11.66 Å

Breadth: 3.887 Å

L/B Ratio: 1.209

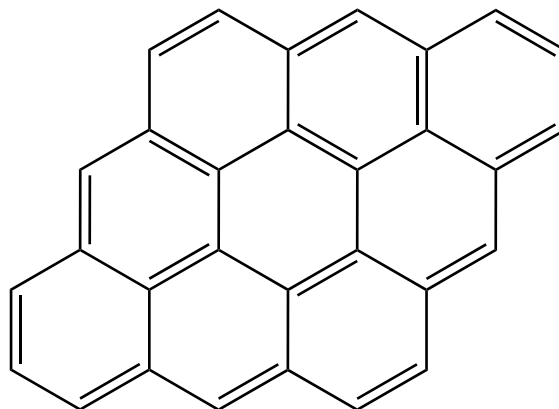
Cartesian coordinates:

C	5.0998	0.4309	0.0000	C	-0.7774	-1.3744	0.0000	H	6.1306	0.0591	0.0000
C	4.8514	1.7978	0.0000	C	-2.9343	3.2555	0.0000	H	5.6894	2.5028	0.0000
C	3.5486	2.2791	0.0000	C	-3.9640	2.3666	0.0000	H	3.3511	3.3622	0.0000
C	4.0359	-0.4756	0.0000	C	-1.5751	2.8073	0.0000	H	3.4198	-3.8582	0.0000
C	3.2390	-2.7770	0.0000	C	-1.3073	1.4282	0.0000	H	5.3058	-2.2493	0.0000
C	4.2667	-1.9000	0.0000	C	0.0368	0.9631	0.0000	H	1.0055	-4.3002	0.0000
C	1.8693	-2.3221	0.0000	C	1.0927	1.8804	0.0000	H	-3.7513	-3.9205	0.0000
C	0.8083	-3.2211	0.0000	C	0.8013	3.2655	0.0000	H	-1.4130	-4.7482	0.0000
C	2.7076	0.0065	0.0000	C	-0.4933	3.7196	0.0000	H	-3.1252	4.3348	0.0000
C	2.4618	1.3989	0.0000	C	-2.1306	-0.9036	0.0000	H	-5.0040	2.7127	0.0000
C	1.6163	-0.9252	0.0000	C	-2.3931	0.4954	0.0000	H	1.6472	3.9706	0.0000
C	-0.5186	-2.7619	0.0000	C	-3.7172	0.9572	0.0000	H	-0.7044	4.7951	0.0000
C	-2.9080	-3.2204	0.0000	C	-4.7802	0.0173	0.0000	H	-5.8117	0.3879	0.0000
C	-1.6277	-3.6733	0.0000	C	-4.5259	-1.3291	0.0000	H	-5.3511	-2.0505	0.0000
C	0.2944	-0.4540	0.0000	C	-3.1935	-1.8156	0.0000				

Table 3.380: Table of thermodynamic data as a function of temperature for Naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-50.012	402.572	402.572	∞
100	101.510	340.068	778.986	-43.892	426.686	466.044	-243.432
200	220.103	444.930	585.353	-28.085	413.855	510.538	-133.336
250	287.367	501.236	562.858	-15.406	407.882	535.398	-111.863
298.15	352.311	557.423	557.423	0.000	402.572	560.454	-98.187
300	354.770	559.609	557.429	0.654	402.375	561.431	-97.752
350	419.366	619.199	561.988	20.024	397.472	588.340	-87.803
400	479.256	679.166	572.887	42.512	393.201	615.895	-80.426
450	533.547	738.806	588.015	67.856	389.478	643.960	-74.747
500	582.099	797.583	606.042	95.770	386.218	672.436	-70.248
600	663.454	911.201	647.515	158.211	380.816	730.213	-63.569
700	727.545	1018.478	692.926	227.886	376.735	788.793	-58.859
800	778.619	1119.087	739.977	303.288	373.836	847.859	-55.358
900	819.924	1213.263	787.390	383.285	371.965	907.217	-52.652
1000	853.783	1301.460	834.435	467.025	370.987	966.749	-50.497
1100	881.853	1384.191	880.692	553.849	370.718	1026.354	-48.736
1200	905.345	1461.960	925.923	643.243	371.036	1085.937	-47.269
1300	925.163	1535.230	970.002	734.796	371.772	1145.488	-46.025
1400	942.002	1604.425	1012.870	828.177	372.805	1204.973	-44.957
1500	956.401	1669.920	1054.510	923.115	374.067	1264.380	-44.029
1600	968.789	1732.050	1094.931	1019.390	375.435	1323.688	-43.213
1700	979.505	1791.112	1134.160	1116.818	376.845	1382.884	-42.490
1800	988.823	1847.369	1172.233	1215.245	378.224	1442.065	-41.847
1900	996.968	1901.055	1209.190	1314.543	379.548	1501.115	-41.268
2000	1004.119	1952.378	1245.076	1414.605	380.770	1560.126	-40.745
2100	1010.427	2001.525	1279.935	1515.339	381.812	1619.064	-40.271
2200	1016.014	2048.662	1313.813	1616.667	382.677	1677.958	-39.839
2300	1020.983	2093.937	1346.754	1718.521	383.364	1736.819	-39.444
2400	1025.419	2137.485	1378.800	1820.845	383.801	1795.601	-39.079
2500	1029.393	2179.427	1409.991	1923.590	384.006	1854.491	-38.747
2600	1032.965	2219.871	1440.367	2026.711	383.941	1913.252	-38.437
2700	1036.187	2258.917	1469.965	2130.171	383.613	1972.103	-38.152
2800	1039.102	2296.654	1498.820	2233.938	382.997	2030.989	-37.888
2900	1041.747	2333.165	1526.964	2337.982	382.063	2089.848	-37.641
3000	1044.153	2368.523	1554.430	2442.279	380.861	2148.774	-37.413
3100	1046.348	2402.797	1581.246	2546.806	379.308	2207.658	-37.198
3200	1048.356	2436.049	1607.442	2651.542	377.450	2266.679	-36.999
3300	1050.196	2468.337	1633.043	2756.471	375.271	2325.808	-36.814
3400	1051.887	2499.714	1658.074	2861.577	372.739	2384.909	-36.639
3500	1053.444	2530.229	1682.559	2966.844	369.861	2444.071	-36.475
3600	1054.881	2559.925	1706.519	3072.262	366.664	2503.420	-36.323
3700	1056.209	2588.846	1729.977	3177.817	363.111	2562.874	-36.181
3800	1057.439	2617.030	1752.951	3283.500	359.179	2622.371	-36.046
3900	1058.581	2644.513	1775.461	3389.302	354.910	2681.912	-35.919
4000	1059.642	2671.327	1797.524	3495.213	350.287	2741.723	-35.802
4100	1060.630	2697.505	1819.157	3601.228	345.275	2801.573	-35.692
4200	1061.551	2723.075	1840.375	3707.337	339.901	2861.541	-35.588
4300	1062.412	2748.064	1861.195	3813.536	334.154	2921.543	-35.489
4400	1063.217	2772.497	1881.630	3919.818	328.041	2981.781	-35.398
4500	1063.971	2796.399	1901.693	4026.178	321.580	3042.220	-35.312
4600	1064.678	2819.792	1921.398	4132.610	314.712	3102.823	-35.233
4700	1065.342	2842.696	1940.758	4239.112	307.458	3163.453	-35.157
4800	1065.966	2865.132	1959.783	4345.677	299.862	3224.358	-35.087
4900	1066.554	2887.118	1978.484	4452.304	291.849	3285.275	-35.021
5000	1067.108	2908.671	1996.873	4558.987	283.517	3346.560	-34.961

3.381. Dibenzo[bc,kl]coronene



Other names: Dibenzo[*ijk,tuv*]peropyrene
2,3,8,9-Dibenzocoronene
anti-diperi-Dibenzocoronene

Formula: C₃₀H₁₄
Mass: 374.432 g/mol
CAS Number: 190-55-6
Point Group: D_{2h}

Length: 15.83 Å
Width: 11.69 Å
Breadth: 3.885 Å
L/B Ratio: 1.355

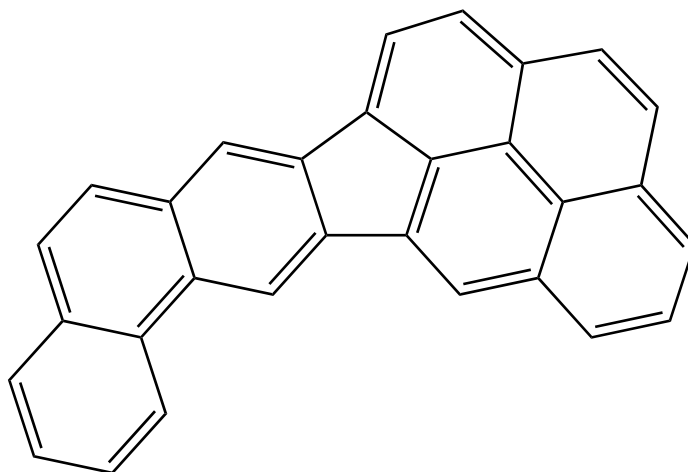
Cartesian coordinates:

C	4.9353	-1.2162	0.0000	C	2.8323	-0.0041	0.0000	H	5.4885	-2.1622	0.0000
C	5.6219	-0.0081	0.0000	C	-3.5356	1.2330	0.0000	H	6.7172	-0.0096	0.0000
C	4.9387	1.2020	0.0000	C	-4.9352	1.2162	0.0000	H	5.4948	2.1463	0.0000
C	3.5391	1.2228	0.0000	C	-5.6219	0.0081	0.0000	H	3.3711	3.3967	0.0000
C	2.8058	2.4567	0.0000	C	-4.9388	-1.2020	0.0000	H	1.2432	4.6412	0.0000
C	1.4399	2.4649	0.0000	C	-2.8323	0.0041	0.0000	H	-1.2298	4.6448	0.0000
C	0.6784	3.7016	0.0000	C	-3.5391	-1.2228	0.0000	H	-3.3613	3.4065	0.0000
C	-0.6677	3.7036	0.0000	C	-2.8058	-2.4567	0.0000	H	3.3613	-3.4065	0.0000
C	-1.4327	2.4691	0.0000	C	-1.4055	0.0020	0.0000	H	-5.4886	2.1622	0.0000
C	-2.7987	2.4648	0.0000	C	-0.7036	-1.2243	0.0000	H	-6.7172	0.0097	0.0000
C	-0.7001	1.2264	0.0000	C	-1.4399	-2.4649	0.0000	H	-5.4947	-2.1464	0.0000
C	0.7036	1.2243	0.0000	C	-0.6783	-3.7016	0.0000	H	-3.3711	-3.3968	0.0000
C	1.4055	-0.0020	0.0000	C	0.6676	-3.7036	0.0000	H	-1.2432	-4.6412	0.0000
C	2.7987	-2.4648	0.0000	C	1.4327	-2.4690	0.0000	H	1.2298	-4.6448	0.0000
C	3.5355	-1.2330	0.0000	C	0.7001	-1.2264	0.0000				

Table 3.381: Table of thermodynamic data as a function of temperature for Dibenzo[bc,kl]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-49.955	455.148	455.148	∞
100	100.286	324.674	764.740	-44.007	479.148	520.045	-271.638
200	220.848	429.367	570.430	-28.213	466.304	566.099	-147.847
250	288.719	485.908	547.829	-15.480	460.384	591.732	-123.633
298.15	354.023	542.367	542.367	0.000	455.148	617.519	-108.184
300	356.492	544.564	542.373	0.657	454.954	618.524	-107.692
350	421.256	604.434	546.954	20.118	450.142	646.178	-96.435
400	481.172	664.657	557.903	42.701	445.967	674.465	-88.074
450	535.405	724.519	573.096	68.140	442.338	703.250	-81.629
500	583.859	783.487	591.196	96.145	439.170	732.436	-76.515
600	664.984	897.406	632.821	158.751	433.932	791.606	-68.914
700	728.863	1004.902	678.377	228.568	429.993	851.554	-63.542
800	779.760	1105.675	725.560	304.092	427.216	911.969	-59.544
900	820.923	1199.977	773.092	384.196	425.453	972.661	-56.451
1000	854.665	1288.274	820.244	468.030	424.568	1033.517	-53.984
1100	882.639	1371.084	866.595	554.938	424.383	1094.437	-51.969
1200	906.048	1448.917	911.912	644.406	424.775	1155.327	-50.289
1300	925.797	1522.241	956.068	736.026	425.578	1216.179	-48.866
1400	942.575	1591.481	999.005	829.466	426.671	1276.961	-47.643
1500	956.921	1657.014	1040.707	924.460	427.988	1337.660	-46.581
1600	969.262	1719.176	1081.186	1020.784	429.405	1398.257	-45.647
1700	979.937	1778.265	1120.467	1118.256	430.860	1458.740	-44.821
1800	989.220	1834.545	1158.587	1216.725	432.280	1519.204	-44.085
1900	997.332	1888.252	1195.588	1316.061	433.643	1579.535	-43.424
2000	1004.455	1939.593	1231.514	1416.158	434.900	1639.825	-42.827
2100	1010.737	1988.756	1266.411	1516.924	435.974	1700.042	-42.285
2200	1016.301	2035.906	1300.324	1618.282	436.868	1760.211	-41.792
2300	1021.250	2081.194	1333.297	1720.164	437.583	1820.348	-41.341
2400	1025.667	2124.753	1365.372	1822.514	438.046	1880.403	-40.925
2500	1029.624	2166.705	1396.592	1925.282	438.274	1940.566	-40.545
2600	1033.181	2207.158	1426.994	2028.426	438.232	2000.599	-40.192
2700	1036.389	2246.211	1456.616	2131.907	437.925	2060.721	-39.866
2800	1039.292	2283.956	1485.494	2235.693	437.328	2120.877	-39.565
2900	1041.925	2320.473	1513.660	2339.756	436.413	2181.005	-39.283
3000	1044.321	2355.836	1541.146	2444.070	435.228	2241.200	-39.022
3100	1046.506	2390.116	1567.982	2548.613	433.691	2301.353	-38.777
3200	1048.505	2423.373	1594.196	2653.365	431.850	2361.642	-38.549
3300	1050.337	2455.666	1619.814	2758.309	429.685	2422.038	-38.337
3400	1052.021	2487.047	1644.862	2863.428	427.166	2482.406	-38.137
3500	1053.571	2517.565	1669.362	2968.708	424.302	2542.835	-37.949
3600	1055.001	2547.265	1693.338	3074.138	421.116	2603.450	-37.774
3700	1056.323	2576.189	1716.810	3179.705	417.575	2664.170	-37.611
3800	1057.548	2604.376	1739.797	3285.399	413.654	2724.932	-37.456
3900	1058.684	2631.861	1762.320	3391.212	409.396	2785.739	-37.310
4000	1059.741	2658.678	1784.395	3497.133	404.784	2846.815	-37.175
4100	1060.724	2684.858	1806.039	3603.157	399.780	2907.930	-37.047
4200	1061.641	2710.430	1827.269	3709.276	394.416	2969.162	-36.926
4300	1062.498	2735.421	1848.100	3815.484	388.678	3030.428	-36.812
4400	1063.299	2759.857	1868.545	3921.774	382.573	3091.930	-36.705
4500	1064.050	2783.761	1888.618	4028.142	376.120	3153.633	-36.606
4600	1064.754	2807.155	1908.333	4134.582	369.260	3215.500	-36.512
4700	1065.415	2830.061	1927.701	4241.091	362.013	3277.394	-36.423
4800	1066.036	2852.498	1946.735	4347.664	354.425	3339.562	-36.341
4900	1066.621	2874.485	1965.445	4454.297	346.418	3401.743	-36.262
5000	1067.173	2896.040	1983.842	4560.987	338.093	3464.290	-36.190

3.382. Naphth[1',2':5,6]indeno[1,2,3-*cd*]pyrene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 106404-28-8
Point Group: C_s

Length: 16.91 Å
Width: 10.41 Å
Breadth: 3.885 Å
L/B Ratio: 1.625

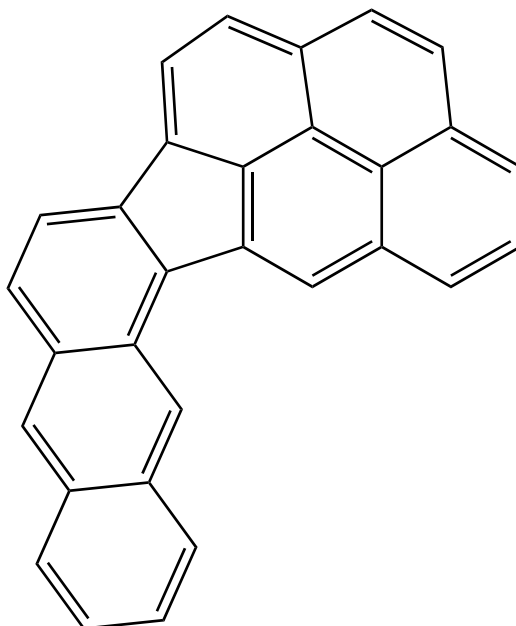
Cartesian coordinates:

C	6.6367	0.7645	0.0000	C	-1.4704	-3.0999	0.0000	H	5.4740	3.9555	0.0000
C	6.6537	2.1395	0.0000	C	-1.6301	-0.7084	0.0000	H	3.2912	2.7495	0.0000
C	5.4469	2.8610	0.0000	C	-0.8565	0.5135	0.0000	H	4.1869	-3.1366	0.0000
C	4.2433	2.1969	0.0000	C	-1.5035	1.7047	0.0000	H	6.3410	-1.9036	0.0000
C	5.4085	0.0659	0.0000	C	-2.9571	1.7235	0.0000	H	1.7194	1.8693	0.0000
C	4.1995	0.7843	0.0000	C	-3.6768	2.9228	0.0000	H	1.7614	-3.1685	0.0000
C	4.2079	-2.0406	0.0000	C	-5.0688	2.9100	0.0000	H	-3.3699	-4.1256	0.0000
C	5.3847	-1.3680	0.0000	C	-5.7864	1.7179	0.0000	H	-0.8877	-4.0267	0.0000
C	2.9569	-1.3386	0.0000	C	-3.6617	-1.9906	0.0000	H	-0.9660	2.6591	0.0000
C	2.9456	0.0670	0.0000	C	-3.0130	-0.7368	0.0000	H	-3.1402	3.8783	0.0000
C	1.7099	0.7688	0.0000	C	-3.6981	0.5140	0.0000	H	-5.6114	3.8617	0.0000
C	1.7403	-2.0730	0.0000	C	-5.1076	0.4960	0.0000	H	-6.8819	1.7339	0.0000
C	0.5574	-1.3887	0.0000	C	-5.7795	-0.7847	0.0000	H	-6.8758	-0.7747	0.0000
C	0.5423	0.0598	0.0000	C	-5.1040	-1.9615	0.0000	H	-5.6384	-2.9180	0.0000
C	-0.8323	-1.8668	0.0000	H	7.5737	0.1960	0.0000				
C	-2.8725	-3.1490	0.0000	H	7.6049	2.6817	0.0000				

Table 3.382: Table of thermodynamic data as a function of temperature for Naphth[1',2':5,6]indeno[1,2,3-cd]pyrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.823	495.958	495.958	∞
100	115.532	360.114	828.143	-46.803	522.629	570.055	-297.760
200	234.180	474.543	622.627	-29.617	508.483	623.125	-162.740
250	302.936	534.135	598.935	-16.200	501.852	652.553	-136.341
298.15	369.765	593.223	593.223	0.000	495.958	682.128	-119.503
300	372.299	595.518	593.230	0.686	495.740	683.281	-118.967
350	438.893	657.961	598.009	20.983	490.315	714.979	-106.703
400	500.620	720.658	609.423	44.494	485.610	747.394	-97.598
450	556.537	782.909	625.248	70.948	481.535	780.366	-90.581
500	606.525	844.185	644.087	100.049	478.000	813.786	-85.014
600	690.331	962.479	687.382	165.058	472.238	881.514	-76.741
700	756.529	1074.061	734.735	237.528	468.014	950.088	-70.895
800	809.507	1178.667	783.760	315.925	465.156	1019.154	-66.543
900	852.566	1276.583	833.139	399.100	463.490	1088.499	-63.174
1000	888.037	1368.304	882.118	486.186	462.854	1157.987	-60.486
1100	917.578	1454.371	930.270	576.511	463.046	1227.508	-58.288
1200	942.399	1535.305	977.351	669.545	463.926	1296.960	-56.454
1300	963.411	1611.590	1023.233	764.864	465.307	1366.330	-54.899
1400	981.317	1683.659	1067.856	862.123	467.055	1435.582	-53.561
1500	996.667	1751.900	1111.205	961.042	469.090	1504.702	-52.397
1600	1009.901	1816.656	1153.289	1061.386	471.276	1573.670	-51.374
1700	1021.369	1878.233	1194.137	1162.963	473.541	1642.473	-50.466
1800	1031.358	1936.902	1233.785	1265.611	475.807	1711.211	-49.657
1900	1040.100	1992.904	1272.276	1369.193	478.043	1779.767	-48.928
2000	1047.785	2046.454	1309.656	1473.596	480.195	1848.236	-48.270
2100	1054.570	2097.743	1345.971	1578.721	482.182	1916.585	-47.671
2200	1060.586	2146.943	1381.268	1684.484	484.004	1984.846	-47.125
2300	1065.939	2194.208	1415.593	1790.816	485.657	2053.028	-46.625
2400	1070.721	2239.677	1448.989	1897.653	487.067	2121.089	-46.163
2500	1075.009	2283.475	1481.497	2004.943	488.247	2189.220	-45.740
2600	1078.865	2325.714	1513.160	2112.640	489.160	2257.181	-45.346
2700	1082.344	2366.497	1544.014	2220.704	489.811	2325.193	-44.983
2800	1085.494	2405.917	1574.096	2329.098	490.174	2393.208	-44.645
2900	1088.352	2444.059	1603.441	2437.793	490.216	2461.158	-44.329
3000	1090.954	2481.000	1632.080	2546.760	489.988	2529.140	-44.035
3100	1093.328	2516.812	1660.045	2655.976	489.404	2597.050	-43.759
3200	1095.500	2551.558	1687.365	2765.419	488.511	2665.066	-43.502
3300	1097.491	2585.300	1714.066	2875.070	487.290	2733.158	-43.261
3400	1099.322	2618.091	1740.175	2984.912	485.710	2801.196	-43.034
3500	1101.007	2649.982	1765.716	3094.930	483.777	2869.265	-42.821
3600	1102.563	2681.020	1790.712	3205.109	481.517	2937.493	-42.621
3700	1104.001	2711.249	1815.185	3315.438	478.894	3005.804	-42.433
3800	1105.334	2740.709	1839.155	3425.906	475.881	3074.127	-42.256
3900	1106.571	2769.437	1862.641	3536.502	472.523	3142.476	-42.088
4000	1107.721	2797.467	1885.663	3647.217	468.803	3211.069	-41.931
4100	1108.791	2824.833	1908.237	3758.043	464.681	3279.678	-41.783
4200	1109.790	2851.565	1930.381	3868.973	460.189	3348.383	-41.642
4300	1110.723	2877.690	1952.108	3979.999	455.311	3417.101	-41.509
4400	1111.596	2903.235	1973.436	4091.116	450.057	3486.037	-41.384
4500	1112.413	2928.225	1994.377	4202.316	444.444	3555.156	-41.266
4600	1113.180	2952.683	2014.944	4313.596	438.414	3624.417	-41.156
4700	1113.900	2976.631	2035.152	4424.951	431.984	3693.687	-41.050
4800	1114.577	3000.089	2055.011	4536.375	425.205	3763.214	-40.951
4900	1115.214	3023.078	2074.534	4647.865	417.994	3832.737	-40.857
5000	1115.815	3045.614	2093.731	4759.417	410.456	3902.615	-40.770

3.383. Naphth[2',1':4,5]indeno[1,2,3-*cd*]pyrene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 106404-29-9
Point Group: C_s

Length: 16.58 Å
Width: 11.12 Å
Breadth: 3.885 Å
L/B Ratio: 1.490

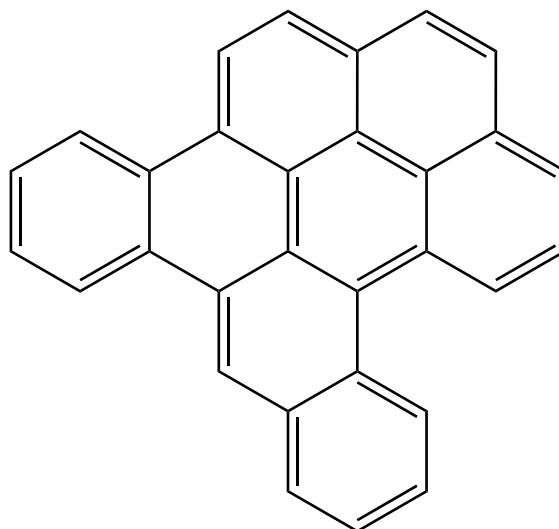
Cartesian coordinates:

C	3.9798	-3.3949	0.0000	C	-0.7206	0.7984	0.0000	H	1.8686	-3.8438	0.0000
C	4.9762	-2.4235	0.0000	C	-0.3794	2.1588	0.0000	H	0.0574	-2.1025	0.0000
C	2.6298	-3.0553	0.0000	C	-1.3735	3.1620	0.0000	H	4.1082	3.8441	0.0000
C	2.2370	-1.7128	0.0000	C	-2.6875	2.7892	0.0000	H	1.6820	4.3712	0.0000
C	0.8366	-1.3251	0.0000	C	-2.0818	0.3876	0.0000	H	6.6607	-0.2853	0.0000
C	3.3824	3.0229	0.0000	C	-3.0756	1.4107	0.0000	H	6.0055	2.1008	0.0000
C	2.0127	3.3275	0.0000	C	-4.4284	1.0501	0.0000	H	-1.0737	4.2150	0.0000
C	2.9163	0.6525	0.0000	C	-2.4657	-0.9581	0.0000	H	-3.4788	3.5480	0.0000
C	3.2613	-0.7309	0.0000	C	-3.8144	-1.3097	0.0000	H	-5.1980	1.8321	0.0000
C	4.6294	-1.0694	0.0000	C	-4.8088	-0.2918	0.0000	H	-1.6865	-1.7384	0.0000
C	5.6023	0.0010	0.0000	C	-6.1911	-0.6743	0.0000	H	-6.9502	0.1162	0.0000
C	5.2463	1.3108	0.0000	C	-6.5449	-1.9867	0.0000	H	-7.5987	-2.2836	0.0000
C	3.8583	1.7036	0.0000	C	-5.5480	-3.0067	0.0000	H	-5.8690	-4.0534	0.0000
C	0.5108	-0.0081	0.0000	C	-4.2279	-2.6830	0.0000	H	-3.4548	-3.4595	0.0000
C	1.5725	0.9738	0.0000	H	4.2642	-4.4529	0.0000				
C	1.0852	2.2937	0.0000	H	6.0318	-2.7169	0.0000				

Table 3.383: Table of thermodynamic data as a function of temperature for Naphth[2',1':4,5]indeno[1,2,3-cd]pyrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.908	524.913	524.913	∞
100	115.496	361.478	830.049	-46.857	551.530	598.820	-312.785
200	234.506	476.024	624.283	-29.652	537.403	651.750	-170.216
250	303.303	535.694	600.564	-16.217	530.790	681.101	-142.305
298.15	370.123	594.846	594.846	0.000	524.913	710.599	-124.491
300	372.656	597.144	594.853	0.687	524.696	711.750	-123.924
350	439.218	659.639	599.637	21.001	519.288	743.365	-110.939
400	500.907	722.377	611.060	44.527	514.598	775.695	-101.293
450	556.790	784.661	626.896	70.994	510.538	808.581	-93.856
500	606.749	845.961	645.747	100.107	507.014	841.912	-87.952
600	690.511	964.292	689.064	165.137	501.272	909.460	-79.174
700	756.676	1075.899	736.438	237.623	497.064	977.851	-72.967
800	809.629	1180.523	785.481	316.033	494.220	1046.733	-68.343
900	852.666	1278.452	834.875	399.219	492.565	1115.892	-64.763
1000	888.120	1370.183	883.869	486.314	491.938	1185.192	-61.907
1100	917.647	1456.257	932.033	576.646	492.138	1254.525	-59.571
1200	942.457	1537.197	979.124	669.687	493.024	1323.788	-57.622
1300	963.460	1613.486	1025.016	765.011	494.411	1392.968	-55.969
1400	981.359	1685.558	1069.647	862.275	496.163	1462.031	-54.548
1500	996.703	1753.801	1113.003	961.198	498.201	1530.961	-53.312
1600	1009.931	1818.560	1155.094	1061.546	500.391	1599.739	-52.225
1700	1021.396	1880.139	1195.947	1163.125	502.659	1668.351	-51.261
1800	1031.382	1938.809	1235.600	1265.776	504.927	1736.899	-50.402
1900	1040.121	1994.812	1274.096	1369.360	507.166	1805.264	-49.629
2000	1047.803	2048.363	1311.481	1473.765	509.320	1873.542	-48.931
2100	1054.587	2099.653	1347.800	1578.891	511.308	1941.700	-48.296
2200	1060.600	2148.854	1383.101	1684.656	513.132	2009.770	-47.717
2300	1065.952	2196.120	1417.429	1790.989	514.786	2077.761	-47.186
2400	1070.733	2241.589	1450.828	1897.828	516.197	2145.631	-46.697
2500	1075.019	2285.387	1483.340	2005.119	517.379	2213.571	-46.249
2600	1078.875	2327.627	1515.005	2112.817	518.293	2281.340	-45.832
2700	1082.353	2368.410	1545.861	2220.882	518.945	2349.161	-45.446
2800	1085.502	2407.831	1575.946	2329.277	519.308	2416.984	-45.088
2900	1088.360	2445.973	1605.293	2437.972	519.352	2484.743	-44.754
3000	1090.961	2482.915	1633.934	2546.940	519.124	2552.534	-44.443
3100	1093.334	2518.726	1661.901	2656.157	518.540	2620.253	-44.150
3200	1095.506	2553.473	1689.223	2765.600	517.648	2688.077	-43.877
3300	1097.497	2587.214	1715.926	2875.252	516.427	2755.978	-43.623
3400	1099.327	2620.005	1742.037	2985.094	514.848	2823.824	-43.382
3500	1101.012	2651.897	1767.579	3095.113	512.916	2891.702	-43.155
3600	1102.567	2682.935	1792.576	3205.293	510.656	2959.738	-42.944
3700	1104.006	2713.165	1817.050	3315.622	508.033	3027.857	-42.745
3800	1105.338	2742.624	1841.022	3426.090	505.022	3095.989	-42.556
3900	1106.575	2771.352	1864.510	3536.687	501.664	3164.146	-42.378
4000	1107.724	2799.383	1887.532	3647.402	497.944	3232.548	-42.212
4100	1108.795	2826.749	1910.108	3758.229	493.822	3300.966	-42.054
4200	1109.793	2853.480	1932.252	3869.159	489.330	3369.479	-41.905
4300	1110.726	2879.605	1953.981	3980.185	484.453	3438.005	-41.763
4400	1111.599	2905.150	1975.309	4091.302	479.199	3506.749	-41.630
4500	1112.416	2930.140	1996.251	4202.503	473.587	3575.677	-41.505
4600	1113.182	2954.599	2016.820	4313.783	467.557	3644.746	-41.387
4700	1113.902	2978.547	2037.028	4425.138	461.127	3713.825	-41.274
4800	1114.579	3002.005	2056.888	4536.562	454.348	3783.160	-41.168
4900	1115.217	3024.994	2076.412	4648.053	447.138	3852.492	-41.067
5000	1115.817	3047.530	2095.609	4759.605	439.600	3922.178	-40.974

3.384. Tribenzo[*a,e,ghi*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-60-1
Point Group: C₁

Length: 13.84 Å
Width: 12.84 Å
Breadth: 5.013 Å
L/B Ratio: 1.078

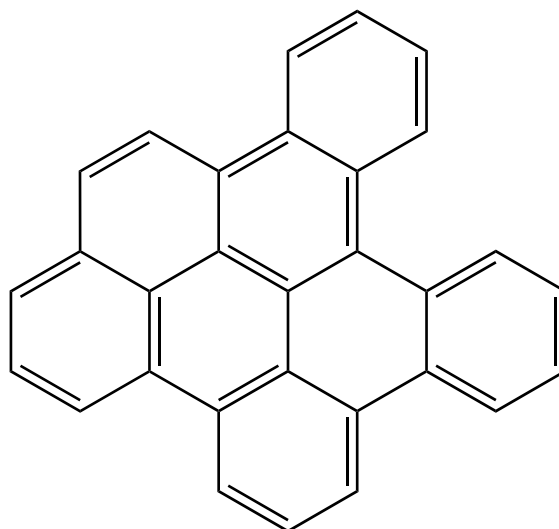
Cartesian coordinates:

C	2.0795	-1.1443	-0.0468	C	-4.0849	0.9315	-0.3215	H	-4.0627	-2.9226	0.0820
C	2.0937	0.2624	-0.2347	C	1.9563	3.2278	0.4657	H	-4.0854	2.0269	-0.4301
C	0.8543	1.0172	-0.0568	C	1.8770	4.5866	0.5998	H	-2.5648	2.9287	-0.2603
C	-0.3579	0.3134	-0.0519	C	0.6512	5.2587	0.3946	H	2.9196	2.7310	0.6444
C	-0.3821	-1.1286	0.0586	C	-0.4743	4.5365	0.1158	H	2.7637	5.1679	0.8739
C	0.8404	-1.8403	0.1381	C	3.2797	-1.8857	-0.1040	H	0.6136	6.3495	0.4775
C	0.8206	2.4410	0.1189	C	4.4804	-1.2439	-0.4415	H	-1.4408	5.0356	-0.0192
C	-0.4161	3.1177	0.0126	C	4.4700	0.1039	-0.7448	H	5.4117	-1.8194	-0.4850
C	-1.6118	2.3861	-0.1506	C	3.2928	0.8446	-0.6455	H	5.3931	0.6019	-1.0601
C	-1.6042	1.0095	-0.1209	C	0.8400	-3.2343	0.3316	H	3.3304	1.9136	-0.8961
C	-1.5904	-1.8366	0.1264	C	-0.3840	-3.9173	0.4457	H	-2.5299	-3.7662	0.3972
C	-2.8543	-1.1316	-0.0205	C	-1.5707	-3.2297	0.3321	H	-0.3844	-5.0006	0.6112
C	-2.8581	0.2651	-0.1594	C	3.2562	-3.2994	0.1576	H	2.0633	-5.0225	0.5773
C	-4.0746	-1.8283	-0.0362	C	2.0873	-3.9452	0.3772	H	4.2105	-3.8384	0.1683
C	-5.2718	-1.1573	-0.1966	H	-6.2245	0.7637	-0.4732				
C	-5.2765	0.2318	-0.3430	H	-6.2160	-1.7112	-0.2101				

Table 3.384: Table of thermodynamic data as a function of temperature for Tribenzo[*a,e,ghi*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.708	485.102	485.102	∞
100	114.986	357.645	825.099	-46.745	511.830	559.503	-292.249
200	234.013	471.992	619.836	-29.569	497.675	612.828	-160.051
250	302.419	531.508	596.186	-16.169	491.026	642.384	-134.216
298.15	369.041	590.485	590.485	0.000	485.102	672.088	-117.745
300	371.571	592.775	590.492	0.685	484.883	673.246	-117.220
350	438.114	655.100	595.262	20.944	479.419	705.085	-105.226
400	499.890	717.696	606.655	44.416	474.676	737.645	-96.325
450	555.900	779.867	622.453	70.836	470.567	770.768	-89.467
500	605.983	841.080	641.265	99.907	467.003	804.341	-84.027
600	689.932	959.290	684.505	164.871	461.194	872.384	-75.946
700	756.195	1070.816	731.809	237.305	456.934	941.280	-70.238
800	809.188	1175.378	780.792	315.669	454.044	1010.673	-65.989
900	852.237	1273.257	830.132	398.812	452.345	1080.349	-62.701
1000	887.694	1364.942	879.078	485.864	451.676	1150.171	-60.078
1100	917.224	1450.975	927.199	576.154	451.833	1220.030	-57.933
1200	942.040	1531.879	974.252	669.152	452.678	1289.823	-56.143
1300	963.053	1608.135	1020.108	764.435	454.023	1359.537	-54.626
1400	980.965	1680.177	1064.706	861.659	455.735	1429.136	-53.321
1500	996.325	1748.394	1108.032	960.543	457.735	1498.606	-52.185
1600	1009.570	1813.129	1150.095	1060.854	459.888	1567.925	-51.186
1700	1021.052	1874.686	1190.922	1162.399	462.120	1637.082	-50.300
1800	1031.056	1933.337	1230.551	1265.015	464.355	1706.176	-49.511
1900	1039.813	1989.324	1269.024	1368.568	466.562	1775.089	-48.800
2000	1047.512	2042.859	1306.388	1472.943	468.686	1843.916	-48.157
2100	1054.312	2094.135	1342.687	1578.041	470.646	1912.626	-47.573
2200	1060.341	2143.324	1377.969	1683.779	472.443	1981.248	-47.040
2300	1065.707	2190.578	1412.280	1790.087	474.072	2049.793	-46.551
2400	1070.502	2236.038	1445.662	1896.902	475.459	2118.217	-46.101
2500	1074.801	2279.826	1478.158	2004.171	476.618	2186.713	-45.688
2600	1078.669	2322.057	1509.808	2111.848	477.511	2255.039	-45.303
2700	1082.158	2362.833	1540.651	2219.892	478.143	2323.417	-44.948
2800	1085.317	2402.247	1570.723	2328.268	478.488	2391.798	-44.619
2900	1088.185	2440.383	1600.057	2436.946	478.513	2460.115	-44.311
3000	1090.795	2477.319	1628.687	2545.897	478.268	2528.466	-44.024
3100	1093.177	2513.125	1656.642	2655.097	477.669	2596.744	-43.754
3200	1095.357	2547.867	1683.953	2764.525	476.761	2665.129	-43.503
3300	1097.355	2581.604	1710.646	2874.162	475.526	2733.590	-43.268
3400	1099.192	2614.391	1736.747	2983.991	473.933	2801.998	-43.047
3500	1100.884	2646.279	1762.280	3093.996	471.988	2870.437	-42.838
3600	1102.445	2677.314	1787.268	3204.163	469.715	2939.036	-42.643
3700	1103.889	2707.539	1811.734	3314.481	467.081	3007.717	-42.460
3800	1105.227	2736.996	1835.697	3424.938	464.057	3076.412	-42.287
3900	1106.468	2765.721	1859.177	3535.523	460.689	3145.132	-42.123
4000	1107.622	2793.749	1882.192	3646.228	456.958	3214.097	-41.971
4100	1108.697	2821.113	1904.760	3757.045	452.827	3283.078	-41.826
4200	1109.700	2847.842	1926.898	3867.965	448.325	3352.155	-41.689
4300	1110.636	2873.965	1948.620	3978.983	443.438	3421.245	-41.559
4400	1111.512	2899.508	1969.942	4090.091	438.176	3490.554	-41.437
4500	1112.333	2924.496	1990.877	4201.283	432.555	3560.046	-41.323
4600	1113.103	2948.952	2011.440	4312.556	426.517	3629.679	-41.215
4700	1113.826	2972.899	2031.643	4423.902	420.080	3699.322	-41.113
4800	1114.506	2996.356	2051.498	4535.319	413.293	3769.223	-41.017
4900	1115.146	3019.343	2071.016	4646.802	406.076	3839.120	-40.925
5000	1115.749	3041.878	2090.208	4758.347	398.531	3909.371	-40.840

3.385. Benzo[*a*]naphtho[2,1,8-*cde*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-66-7
Point Group: C₁

Length: 13.70 Å
Width: 11.85 Å
Breadth: 5.213 Å
L/B Ratio: 1.156

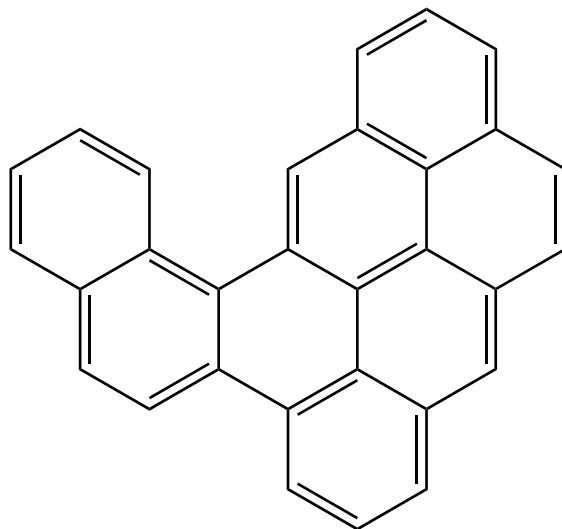
Cartesian coordinates:

C	1.4619	2.1061	0.2009	C	2.1431	-2.9306	-0.3357	H	-1.6524	4.4203	0.5325
C	1.6145	3.4719	0.4228	C	3.3868	-2.3902	-0.4097	H	5.7314	-1.0701	-0.4448
C	0.5020	4.2990	0.5649	C	-2.4416	0.4625	-0.1967	H	6.0296	1.3856	-0.1817
C	-0.7684	3.7699	0.4504	C	-2.2746	1.8495	-0.0196	H	4.0534	2.8608	0.1325
C	-0.0290	0.1192	0.0117	C	-3.3830	2.7115	-0.1428	H	1.9960	-4.0182	-0.4181
C	0.1634	1.5464	0.1268	C	-4.6196	2.2293	-0.5103	H	4.2685	-3.0229	-0.5627
C	-0.9534	2.3979	0.2110	C	-4.7699	0.8664	-0.7893	H	-3.2400	3.7861	0.0481
C	-1.3079	-0.4313	-0.0038	C	-3.7028	0.0072	-0.6357	H	-5.4753	2.9056	-0.6033
C	2.6308	1.2505	0.0365	C	-0.3129	-2.6924	0.0409	H	-5.7376	0.4853	-1.1317
C	4.8638	-0.4148	-0.3075	C	-1.4443	-1.8606	0.1725	H	-3.8447	-1.0576	-0.8657
C	5.0279	0.9439	-0.1622	C	-2.6648	-2.4736	0.5517	H	-3.5452	-1.8454	0.7447
C	3.9139	1.7754	0.0122	C	-2.7775	-3.8346	0.6935	H	-3.7314	-4.2821	0.9916
C	3.5709	-0.9792	-0.2768	C	-1.6668	-4.6632	0.4605	H	-1.7709	-5.7496	0.5448
C	2.4443	-0.1488	-0.1073	C	-0.4565	-4.0970	0.1505	H	0.4301	-4.7297	-0.0073
C	1.1315	-0.7248	-0.0700	H	2.6290	3.8950	0.4837				
C	0.9890	-2.1094	-0.1408	H	0.6394	5.3683	0.7553				

Table 3.385: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[2,1,8-*cde*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.694	487.706	487.706	∞
100	115.292	356.249	823.672	-46.742	514.438	562.251	-293.684
200	233.985	470.746	618.477	-29.546	500.302	615.704	-160.802
250	302.170	530.231	594.847	-16.154	493.646	645.324	-134.830
298.15	368.666	589.151	589.151	0.000	487.706	675.090	-118.271
300	371.193	591.439	589.158	0.684	487.487	676.251	-117.743
350	437.686	653.702	593.923	20.922	482.003	708.158	-105.685
400	499.459	716.239	605.305	44.374	477.238	740.789	-96.735
450	555.487	778.360	621.089	70.772	473.108	773.986	-89.840
500	605.597	839.531	639.884	99.823	469.524	807.636	-84.371
600	689.595	957.675	683.091	164.751	463.679	875.837	-76.247
700	755.890	1069.152	730.362	237.153	459.387	944.897	-70.508
800	808.903	1173.675	779.315	315.488	456.468	1014.459	-66.236
900	851.967	1271.521	828.629	398.603	454.741	1084.306	-62.930
1000	887.436	1363.179	877.550	485.628	454.045	1154.304	-60.293
1100	916.977	1449.188	925.649	575.893	454.177	1224.340	-58.138
1200	941.805	1530.070	972.681	668.867	454.997	1294.313	-56.339
1300	962.831	1606.308	1018.517	764.127	456.320	1364.209	-54.813
1400	980.755	1678.335	1063.099	861.330	458.010	1433.992	-53.502
1500	996.127	1746.537	1106.408	960.194	459.990	1503.646	-52.361
1600	1009.385	1811.259	1148.456	1060.485	462.123	1573.152	-51.357
1700	1020.879	1872.806	1189.270	1162.012	464.338	1642.496	-50.467
1800	1030.893	1931.448	1228.886	1264.612	466.556	1711.779	-49.673
1900	1039.660	1987.425	1267.347	1368.149	468.747	1780.881	-48.959
2000	1047.370	2040.953	1304.699	1472.509	470.857	1849.899	-48.313
2100	1054.178	2092.222	1340.988	1577.593	472.803	1918.799	-47.727
2200	1060.215	2141.405	1376.260	1683.319	474.587	1987.613	-47.191
2300	1065.590	2188.654	1410.561	1789.614	476.204	2056.350	-46.700
2400	1070.392	2234.109	1443.935	1896.417	477.580	2124.967	-46.248
2500	1074.697	2277.893	1476.423	2003.676	478.728	2193.655	-45.833
2600	1078.571	2320.120	1508.065	2111.343	479.611	2262.175	-45.447
2700	1082.066	2360.893	1538.901	2219.377	480.233	2330.747	-45.090
2800	1085.231	2400.303	1568.965	2327.745	480.569	2399.323	-44.759
2900	1088.103	2438.436	1598.293	2436.414	480.586	2467.834	-44.450
3000	1090.718	2475.369	1626.917	2545.357	480.333	2536.380	-44.161
3100	1093.104	2511.173	1654.867	2654.550	479.726	2604.853	-43.891
3200	1095.287	2545.913	1682.172	2763.971	478.811	2673.433	-43.638
3300	1097.289	2579.647	1708.859	2873.601	477.569	2742.090	-43.403
3400	1099.129	2612.433	1734.955	2983.423	475.969	2810.693	-43.180
3500	1100.824	2644.318	1760.483	3093.422	474.018	2879.329	-42.971
3600	1102.388	2675.352	1785.467	3203.584	471.740	2948.123	-42.775
3700	1103.835	2705.576	1809.929	3313.896	469.100	3017.001	-42.592
3800	1105.175	2735.031	1833.887	3424.347	466.071	3085.892	-42.418
3900	1106.419	2763.755	1857.363	3534.928	462.698	3154.809	-42.253
4000	1107.575	2791.782	1880.375	3645.628	458.962	3223.970	-42.100
4100	1108.652	2819.144	1902.939	3756.440	454.826	3293.148	-41.954
4200	1109.657	2845.872	1925.073	3867.356	450.320	3362.422	-41.817
4300	1110.595	2871.994	1946.792	3978.369	445.429	3431.710	-41.686
4400	1111.473	2897.536	1968.111	4089.473	440.163	3501.215	-41.564
4500	1112.295	2922.524	1989.043	4200.662	434.538	3570.904	-41.449
4600	1113.066	2946.979	2009.603	4311.930	428.497	3640.735	-41.341
4700	1113.791	2970.925	2029.803	4423.274	422.056	3710.576	-41.238
4800	1114.472	2994.381	2049.655	4534.687	415.265	3780.674	-41.141
4900	1115.114	3017.368	2069.170	4646.167	408.045	3850.768	-41.049
5000	1115.718	3039.902	2088.360	4757.709	400.497	3921.217	-40.964

3.386. Dibenzo[*c,hi*]naphtho[3,2,1,8-*mno*p]chrysene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-72-5
Point Group: C₁

Length: 14.38 Å
Width: 12.53 Å
Breadth: 5.079 Å
L/B Ratio: 1.148

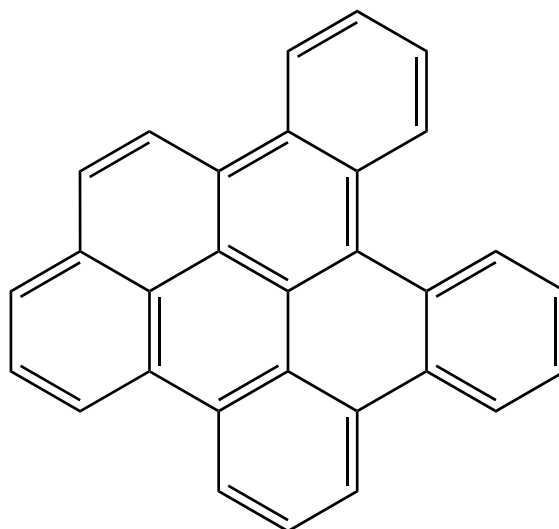
Cartesian coordinates:

C	-3.1110	3.8969	0.4594	C	-2.4402	1.2152	0.0660	H	-1.0063	4.2483	0.7437
C	-4.1186	2.9610	0.1884	C	-3.7980	1.6257	-0.0046	H	0.6876	2.5135	0.5557
C	-1.7892	3.5117	0.5305	C	-4.8114	0.6271	-0.2675	H	-1.9314	-5.0084	-0.2958
C	-1.4302	2.1621	0.3258	C	-4.4889	-0.6749	-0.3992	H	0.4163	-5.7361	0.0763
C	-0.0692	1.7415	0.3530	C	1.6967	-0.0045	0.0769	H	2.2184	-4.0671	0.3741
C	0.2996	0.4392	0.1177	C	1.9699	-1.3600	0.2478	H	-3.5818	-3.2192	-0.5020
C	0.9151	-2.3646	0.1585	C	3.3026	-1.7995	0.4855	H	-5.8508	0.9651	-0.3500
C	-1.1327	-4.2700	-0.1630	C	4.3440	-0.9236	0.4839	H	-5.2595	-1.4305	-0.5916
C	0.1657	-4.6706	0.0420	C	2.8083	0.8917	-0.1239	H	3.4751	-2.8683	0.6841
C	1.1866	-3.7224	0.2082	C	4.1208	0.4349	0.1307	H	5.3624	-1.2562	0.7146
C	-1.4535	-2.8930	-0.1917	C	5.2297	1.3103	-0.0089	H	6.2305	0.9380	0.2389
C	-0.4257	-1.9363	-0.0359	C	5.0523	2.5905	-0.4587	H	5.9026	3.2709	-0.5690
C	-0.7412	-0.5475	-0.0232	C	3.7583	3.0322	-0.8038	H	3.6289	4.0407	-1.2107
C	-2.8001	-2.4649	-0.3492	C	2.6753	2.2093	-0.6412	H	1.6809	2.5752	-0.9317
C	-3.1182	-1.1305	-0.2866	H	-3.3846	4.9459	0.6153				
C	-2.0847	-0.1563	-0.0906	H	-5.1629	3.2885	0.1341				

Table 3.386: Table of thermodynamic data as a function of temperature for Dibenzoc[*c,hi*]naphtho[3,2,1,8-*mno*p]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.502	494.531	494.531	∞
100	113.506	355.554	821.983	-46.643	521.362	569.245	-297.337
200	233.575	469.124	616.985	-29.572	507.101	622.827	-162.662
250	302.500	528.603	593.326	-16.181	500.445	652.529	-136.336
298.15	369.398	587.620	587.620	0.000	494.531	682.372	-119.546
300	371.934	589.913	587.627	0.686	494.313	683.535	-119.012
350	438.587	652.304	592.402	20.966	488.871	715.516	-106.783
400	500.377	714.964	603.807	44.463	484.152	748.214	-97.705
450	556.358	777.191	619.622	70.906	480.067	781.472	-90.709
500	606.399	838.450	638.451	99.999	476.525	815.178	-85.159
600	690.269	956.728	681.728	165.000	470.754	883.480	-76.912
700	756.480	1068.302	729.067	237.465	466.524	952.629	-71.085
800	809.442	1172.900	778.080	315.856	463.661	1022.272	-66.746
900	852.474	1270.808	827.448	399.023	461.987	1092.194	-63.388
1000	887.919	1362.518	876.419	486.099	461.340	1162.260	-60.709
1100	917.438	1448.572	924.562	576.410	461.520	1232.360	-58.519
1200	942.244	1529.493	971.635	669.429	462.385	1302.393	-56.691
1300	963.248	1605.765	1017.509	764.733	463.750	1372.344	-55.140
1400	981.149	1677.822	1062.125	861.976	465.481	1442.180	-53.807
1500	996.499	1746.051	1105.466	960.877	467.499	1511.884	-52.647
1600	1009.734	1810.796	1147.543	1061.205	469.668	1581.437	-51.628
1700	1021.207	1872.363	1188.384	1162.766	471.917	1650.827	-50.723
1800	1031.201	1931.023	1228.025	1265.397	474.167	1720.153	-49.917
1900	1039.949	1987.017	1266.510	1368.964	476.388	1789.297	-49.190
2000	1047.640	2040.559	1303.883	1473.352	478.525	1858.355	-48.534
2100	1054.432	2091.841	1340.193	1578.462	480.498	1927.294	-47.938
2200	1060.454	2141.035	1375.484	1684.213	482.306	1996.145	-47.394
2300	1065.814	2188.295	1409.803	1790.531	483.946	2064.918	-46.895
2400	1070.602	2233.759	1443.194	1897.356	485.344	2133.571	-46.435
2500	1074.895	2277.551	1475.697	2004.635	486.512	2202.294	-46.013
2600	1078.757	2319.786	1507.355	2112.321	487.414	2270.848	-45.621
2700	1082.242	2360.565	1538.204	2220.374	488.055	2339.453	-45.259
2800	1085.396	2399.982	1568.282	2328.758	488.408	2408.061	-44.922
2900	1088.260	2438.120	1597.623	2437.443	488.441	2476.604	-44.608
3000	1090.866	2475.059	1626.258	2546.402	488.203	2545.181	-44.315
3100	1093.244	2510.867	1654.219	2655.609	487.610	2613.685	-44.039
3200	1095.420	2545.611	1681.535	2765.044	486.709	2682.295	-43.783
3300	1097.415	2579.350	1708.233	2874.687	485.480	2750.982	-43.544
3400	1099.249	2612.139	1734.338	2984.522	483.893	2819.615	-43.317
3500	1100.938	2644.028	1759.876	3094.532	481.953	2888.280	-43.104
3600	1102.497	2675.065	1784.869	3204.705	479.686	2957.103	-42.906
3700	1103.938	2705.292	1809.339	3315.027	477.057	3026.009	-42.719
3800	1105.274	2734.750	1833.305	3425.489	474.038	3094.929	-42.542
3900	1106.513	2763.476	1856.789	3536.079	470.674	3163.873	-42.374
4000	1107.665	2791.505	1879.808	3646.789	466.948	3233.062	-42.219
4100	1108.739	2818.870	1902.380	3757.609	462.821	3302.268	-42.071
4200	1109.739	2845.600	1924.520	3868.534	458.323	3371.570	-41.931
4300	1110.674	2871.724	1946.246	3979.555	453.441	3440.884	-41.798
4400	1111.549	2897.268	1967.571	4090.667	448.182	3510.416	-41.673
4500	1112.368	2922.257	1988.509	4201.863	442.564	3580.132	-41.556
4600	1113.136	2946.714	2009.075	4313.139	436.530	3649.990	-41.446
4700	1113.858	2970.661	2029.280	4424.489	430.096	3719.857	-41.341
4800	1114.537	2994.119	2049.138	4535.909	423.312	3789.981	-41.243
4900	1115.176	3017.106	2068.658	4647.395	416.098	3860.101	-41.148
5000	1115.778	3039.642	2087.853	4758.943	408.556	3930.577	-41.062

3.387. Benzo[*b*]naphtho[1,2,3,4-*pqr*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 53156-62-0
Point Group: C₁

Length: 13.70 Å
Width: 11.85 Å
Breadth: 5.213 Å
L/B Ratio: 1.156

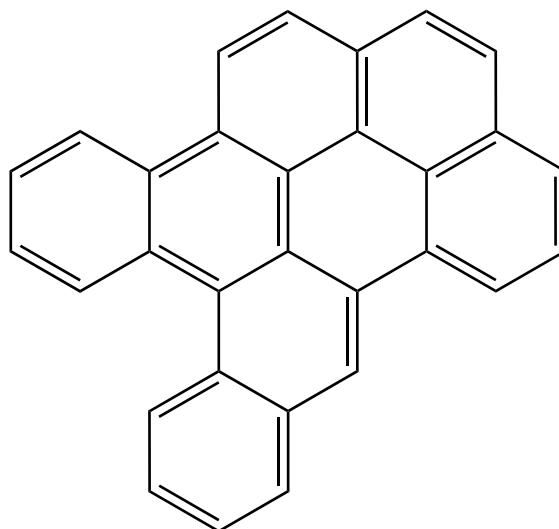
Cartesian coordinates:

C	1.4616	2.1062	0.2011	C	2.1433	-2.9304	-0.3355	H	-1.6528	4.4201	0.5332
C	1.6141	3.4719	0.4235	C	3.3870	-2.3899	-0.4097	H	5.7313	-1.0696	-0.4456
C	0.5016	4.2988	0.5657	C	-0.3127	-2.6924	0.0411	H	6.0293	1.3864	-0.1826
C	-0.7689	3.7697	0.4509	C	-1.4443	-1.8608	0.1725	H	4.0531	2.8612	0.1321
C	-0.0292	0.1191	0.0118	C	-2.6647	-2.4741	0.5514	H	1.9966	-4.0181	-0.4177
C	0.1633	1.5464	0.1269	C	-2.7771	-3.8352	0.6935	H	4.2688	-3.0225	-0.5628
C	-0.9537	2.3978	0.2112	C	-1.6661	-4.6635	0.4609	H	-3.5449	-1.8457	0.7444
C	-1.3080	-0.4314	-0.0039	C	-0.4559	-4.0970	0.1508	H	-3.7310	-4.2826	0.9915
C	2.6306	1.2507	0.0364	C	-2.4417	0.4623	-0.1968	H	-1.7698	-5.7499	0.5454
C	4.8638	-0.4142	-0.3081	C	-2.2748	1.8493	-0.0196	H	0.4309	-4.7296	-0.0067
C	5.0277	0.9444	-0.1629	C	-3.3830	2.7113	-0.1429	H	-3.2401	3.7860	0.0479
C	3.9136	1.7758	0.0118	C	-4.6196	2.2293	-0.5108	H	-5.4751	2.9056	-0.6040
C	3.5709	-0.9789	-0.2770	C	-4.7699	0.8664	-0.7898	H	-5.7375	0.4852	-1.1325
C	2.4443	-0.1485	-0.1074	C	-3.7030	0.0071	-0.6360	H	-3.8441	-1.0578	-0.8660
C	1.1315	-0.7247	-0.0699	H	2.6286	3.8951	0.4845				
C	0.9892	-2.1093	-0.1405	H	0.6389	5.3682	0.7565				

Table 3.387: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[1,2,3,4-*pqr*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.692	487.666	487.666	∞
100	115.282	356.156	823.585	-46.743	514.397	562.219	-293.667
200	233.989	470.649	618.385	-29.547	500.260	615.682	-160.796
250	302.180	530.136	594.754	-16.155	493.605	645.306	-134.827
298.15	368.681	589.058	589.058	0.000	487.666	675.077	-118.268
300	371.207	591.347	589.065	0.684	487.446	676.238	-117.741
350	437.703	653.612	593.831	20.923	481.963	708.150	-105.683
400	499.477	716.152	605.213	44.375	477.199	740.786	-96.735
450	555.506	778.275	620.998	70.775	473.070	773.987	-89.840
500	605.616	839.448	639.794	99.827	469.487	807.641	-84.372
600	689.612	957.595	683.001	164.756	463.644	875.850	-76.248
700	755.907	1069.075	730.275	237.160	459.354	944.918	-70.509
800	808.919	1173.599	779.229	315.496	456.436	1014.487	-66.238
900	851.982	1271.447	828.544	398.613	454.711	1084.342	-62.932
1000	887.450	1363.107	877.466	485.640	454.016	1154.347	-60.296
1100	916.990	1449.117	925.566	575.906	454.150	1224.391	-58.140
1200	941.817	1530.000	972.599	668.881	454.971	1294.371	-56.341
1300	962.842	1606.239	1018.437	764.143	456.294	1364.273	-54.816
1400	980.765	1678.266	1063.019	861.347	457.986	1434.063	-53.504
1500	996.137	1746.470	1106.329	960.211	459.967	1503.724	-52.363
1600	1009.394	1811.192	1148.378	1060.504	462.101	1573.236	-51.360
1700	1020.887	1872.740	1189.192	1162.031	464.317	1642.587	-50.470
1800	1030.901	1931.382	1228.809	1264.632	466.535	1711.877	-49.676
1900	1039.667	1987.360	1267.270	1368.170	468.727	1780.986	-48.962
2000	1047.376	2040.888	1304.623	1472.530	470.838	1850.010	-48.316
2100	1054.184	2092.158	1340.912	1577.615	472.784	1918.917	-47.729
2200	1060.221	2141.340	1376.185	1683.341	474.569	1987.737	-47.194
2300	1065.595	2188.590	1410.487	1789.637	476.187	2056.480	-46.703
2400	1070.397	2234.045	1443.861	1896.441	477.563	2125.104	-46.251
2500	1074.702	2277.829	1476.349	2003.700	478.711	2193.799	-45.836
2600	1078.575	2320.057	1507.992	2111.367	479.595	2262.325	-45.450
2700	1082.071	2360.829	1538.828	2219.402	480.218	2330.903	-45.093
2800	1085.234	2400.239	1568.893	2327.770	480.554	2399.485	-44.762
2900	1088.107	2438.373	1598.221	2436.439	480.571	2468.003	-44.453
3000	1090.721	2475.306	1626.845	2545.383	480.319	2536.555	-44.164
3100	1093.107	2511.110	1654.795	2654.576	479.712	2605.035	-43.894
3200	1095.290	2545.850	1682.100	2763.998	478.797	2673.621	-43.641
3300	1097.292	2579.585	1708.788	2873.628	477.556	2742.284	-43.406
3400	1099.132	2612.370	1734.884	2983.451	475.956	2810.893	-43.183
3500	1100.827	2644.256	1760.413	3093.450	474.005	2879.535	-42.974
3600	1102.391	2675.289	1785.397	3203.612	471.727	2948.336	-42.778
3700	1103.837	2705.513	1809.858	3313.924	469.087	3017.220	-42.595
3800	1105.177	2734.969	1833.817	3424.375	466.059	3086.118	-42.421
3900	1106.421	2763.693	1857.294	3534.956	462.686	3155.040	-42.256
4000	1107.577	2791.720	1880.305	3645.657	458.950	3224.208	-42.103
4100	1108.654	2819.082	1902.870	3756.469	454.815	3293.392	-41.957
4200	1109.659	2845.810	1925.004	3867.385	450.309	3362.673	-41.820
4300	1110.597	2871.932	1946.723	3978.398	445.418	3431.966	-41.689
4400	1111.475	2897.474	1968.042	4089.503	440.152	3501.478	-41.567
4500	1112.297	2922.462	1988.975	4200.692	434.527	3571.173	-41.452
4600	1113.068	2946.917	2009.534	4311.960	428.486	3641.010	-41.344
4700	1113.792	2970.863	2029.734	4423.304	422.045	3710.857	-41.241
4800	1114.474	2994.319	2049.586	4534.717	415.255	3780.961	-41.144
4900	1115.115	3017.305	2069.102	4646.197	408.035	3851.061	-41.052
5000	1115.719	3039.840	2088.292	4757.739	400.487	3921.517	-40.967

3.388. Tribenzo[*b,e,ghi*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-62-3
Point Group: C₁

Length: 14.16 Å
Width: 12.08 Å
Breadth: 5.031 Å
L/B Ratio: 1.172

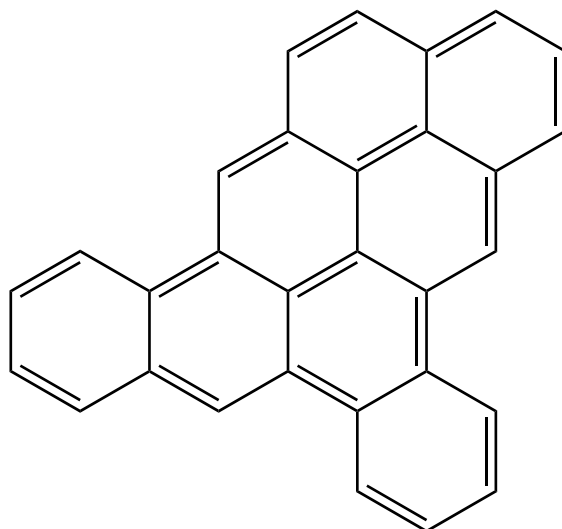
Cartesian coordinates:

C	0.4166	2.6378	0.2048	C	-2.8732	-1.9023	-0.3041	H	-0.4664	-4.3185	-0.5142
C	-0.3816	1.5221	0.1572	C	-2.0502	-0.7829	-0.1132	H	-1.8123	3.7886	0.5292
C	-2.2865	-3.1785	-0.4707	C	1.8161	2.5357	0.0128	H	-4.2861	4.0008	0.5739
C	-0.9266	-3.3246	-0.4052	C	2.4189	1.2677	-0.1368	H	-5.7265	1.9994	0.2514
C	0.2196	0.2253	0.0467	C	3.7879	1.2460	-0.5182	H	-5.9544	-0.4044	-0.1438
C	-0.6345	-0.9320	-0.0711	C	4.5181	2.3984	-0.6446	H	-4.9169	-2.6370	-0.4762
C	-0.0809	-2.2106	-0.1810	C	3.9246	3.6535	-0.3966	H	4.2729	0.2833	-0.7298
C	1.6127	0.0857	0.0285	C	2.5943	3.7204	-0.0831	H	5.5703	2.3550	-0.9447
C	-1.8351	1.6584	0.2148	C	2.1699	-1.2513	0.1800	H	4.5301	4.5621	-0.4742
C	-2.4413	2.8943	0.4014	C	1.3440	-2.3791	0.0037	H	2.1072	4.6878	0.0855
C	-3.8348	3.0148	0.4214	C	1.8968	-3.6742	0.0830	H	1.2438	-4.5399	-0.1065
C	-4.6348	1.9055	0.2450	C	3.2211	-3.8619	0.4081	H	3.6421	-4.8706	0.4671
C	-2.6478	0.5108	0.0526	C	4.0231	-2.7497	0.6893	H	5.0630	-2.8944	1.0000
C	-4.0507	0.6384	0.0548	C	3.5049	-1.4776	0.5788	H	4.1526	-0.6227	0.8164
C	-4.8652	-0.5268	-0.1409	H	-0.0375	3.6322	0.3468				
C	-4.2988	-1.7453	-0.3206	H	-2.9333	-4.0464	-0.6423				

Table 3.388: Table of thermodynamic data as a function of temperature for Tribenzo[*b,e,ghi*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	–53.572	482.422	482.422	∞
100	114.641	356.242	822.792	–46.655	509.241	557.054	–290.969
200	233.540	470.314	617.909	–29.519	495.045	610.533	–159.452
250	301.909	529.720	594.297	–16.144	488.371	640.176	–133.755
298.15	368.512	588.604	588.604	0.000	482.422	669.969	–117.373
300	371.041	590.892	588.612	0.684	482.202	671.130	–116.852
350	437.578	653.135	593.375	20.916	476.712	703.065	–104.925
400	499.361	715.659	604.754	44.362	471.942	735.725	–96.074
450	555.387	777.768	620.534	70.756	467.807	768.952	–89.256
500	605.494	838.928	639.325	99.802	464.217	802.631	–83.849
600	689.500	957.054	682.522	164.719	458.363	870.894	–75.816
700	755.823	1068.518	729.786	237.113	454.063	940.016	–70.143
800	808.871	1173.034	778.731	315.443	451.138	1009.642	–65.922
900	851.969	1270.879	828.038	398.556	449.410	1079.554	–62.654
1000	887.466	1362.538	876.954	485.584	448.715	1149.615	–60.049
1100	917.029	1448.551	925.049	575.852	448.852	1219.716	–57.918
1200	941.872	1529.439	972.078	668.833	449.678	1289.752	–56.140
1300	962.908	1605.682	1017.913	764.100	451.008	1359.710	–54.633
1400	980.838	1677.715	1062.493	861.311	452.706	1429.555	–53.336
1500	996.213	1745.923	1105.801	960.183	454.694	1499.272	–52.208
1600	1009.472	1810.651	1147.849	1060.483	456.837	1568.838	–51.216
1700	1020.965	1872.203	1188.663	1162.018	459.060	1638.243	–50.336
1800	1030.978	1930.849	1228.279	1264.627	461.286	1707.586	–49.552
1900	1039.743	1986.831	1266.741	1368.172	463.486	1776.748	–48.845
2000	1047.449	2040.363	1304.093	1472.540	465.604	1845.825	–48.207
2100	1054.254	2091.637	1340.383	1577.632	467.558	1914.784	–47.627
2200	1060.288	2140.823	1375.657	1683.365	469.349	1983.656	–47.097
2300	1065.660	2188.075	1409.959	1789.668	470.973	2052.451	–46.612
2400	1070.458	2233.532	1443.333	1896.478	472.356	2121.126	–46.164
2500	1074.761	2277.319	1475.822	2003.743	473.511	2189.872	–45.754
2600	1078.631	2319.549	1507.466	2111.416	474.399	2258.449	–45.372
2700	1082.124	2360.324	1538.303	2219.457	475.028	2327.078	–45.019
2800	1085.285	2399.736	1568.368	2327.830	475.369	2395.710	–44.692
2900	1088.155	2437.871	1597.697	2436.504	475.392	2464.279	–44.386
3000	1090.767	2474.806	1626.322	2545.452	475.144	2532.880	–44.100
3100	1093.151	2510.611	1654.273	2654.650	474.541	2601.410	–43.833
3200	1095.332	2545.352	1681.579	2764.075	473.631	2670.046	–43.583
3300	1097.332	2579.089	1708.267	2873.710	472.394	2738.759	–43.350
3400	1099.170	2611.875	1734.364	2983.537	470.798	2807.418	–43.130
3500	1100.863	2643.762	1759.894	3093.539	468.851	2876.109	–42.923
3600	1102.426	2674.796	1784.878	3203.705	466.576	2944.959	–42.729
3700	1103.871	2705.022	1809.340	3314.021	463.940	3013.893	–42.548
3800	1105.209	2734.478	1833.300	3424.475	460.915	3082.839	–42.376
3900	1106.452	2763.203	1856.777	3535.059	457.545	3151.811	–42.213
4000	1107.607	2791.230	1879.790	3645.763	453.812	3221.028	–42.061
4100	1108.682	2818.593	1902.355	3756.578	449.680	3290.261	–41.918
4200	1109.686	2845.322	1924.489	3867.497	445.177	3359.590	–41.782
4300	1110.623	2871.445	1946.209	3978.513	440.289	3428.932	–41.652
4400	1111.500	2896.987	1967.528	4089.619	435.025	3498.493	–41.532
4500	1112.321	2921.975	1988.462	4200.811	429.403	3568.237	–41.418
4600	1113.091	2946.431	2009.022	4312.082	423.364	3638.122	–41.311
4700	1113.815	2970.378	2029.223	4423.428	416.925	3708.018	–41.209
4800	1114.495	2993.834	2049.075	4534.843	410.137	3778.170	–41.114
4900	1115.136	3016.821	2068.591	4646.325	402.919	3848.319	–41.023
5000	1115.739	3039.356	2087.782	4757.869	395.373	3918.823	–40.939

3.389. Benzo[*h*]naphtho[7,8,1,2,3-*pqrst*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-69-0
Point Group: C_s

Length: 15.87 Å
Width: 12.90 Å
Breadth: 3.888 Å
L/B Ratio: 1.231

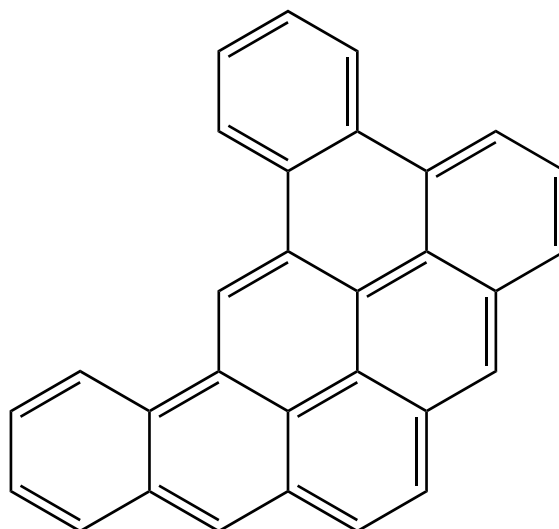
Cartesian coordinates:

C	4.7114	-3.0452	0.0000	C	-5.6076	-0.3713	0.0000	H	5.7054	0.2165	0.0000
C	5.5674	-1.9289	0.0000	C	-5.0920	-1.6691	0.0000	H	2.6683	-3.7381	0.0000
C	5.0446	-0.6578	0.0000	C	-2.8420	-0.7618	0.0000	H	3.7878	1.7149	0.0000
C	3.3478	-2.8722	0.0000	C	-3.7160	-1.8773	0.0000	H	-2.8939	2.6754	0.0000
C	2.7857	-1.5756	0.0000	C	-3.1495	-3.2061	0.0000	H	0.8954	-3.4813	0.0000
C	3.6438	-0.4620	0.0000	C	-1.8130	-3.3943	0.0000	H	-5.1774	1.7406	0.0000
C	3.0960	0.8569	0.0000	C	-0.8973	-2.2758	0.0000	H	-6.6929	-0.2244	0.0000
C	1.7453	1.0694	0.0000	C	-1.4251	-0.9533	0.0000	H	-5.7739	-2.5270	0.0000
C	-1.1146	1.4825	0.0000	C	-0.2009	2.6238	0.0000	H	-3.8409	-4.0567	0.0000
C	-2.4716	1.6574	0.0000	C	1.1901	2.4224	0.0000	H	-1.3849	-4.4033	0.0000
C	-0.5588	0.1526	0.0000	C	2.0409	3.5367	0.0000	H	3.1298	3.3742	0.0000
C	0.4715	-2.4641	0.0000	C	1.5302	4.8243	0.0000	H	2.2086	5.6835	0.0000
C	1.3567	-1.3659	0.0000	C	0.1513	5.0235	0.0000	H	-0.2564	6.0396	0.0000
C	0.8442	-0.0542	0.0000	C	-0.7026	3.9329	0.0000	H	-1.7931	4.0837	0.0000
C	-3.3706	0.5461	0.0000	H	5.1406	-4.0524	0.0000				
C	-4.7649	0.7255	0.0000	H	6.6514	-2.0823	0.0000				

Table 3.389: Table of thermodynamic data as a function of temperature for Benzo[*h*]naphtho[7,8,1,2,3-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	–54.190	467.264	467.264	∞
100	117.135	368.004	837.410	–46.941	493.797	540.434	–282.288
200	234.894	483.406	631.503	–29.619	479.786	592.656	–154.783
250	302.916	543.076	607.819	–16.186	473.172	621.638	–129.881
298.15	369.238	602.113	602.113	0.000	467.264	650.783	–114.012
300	371.757	604.405	602.120	0.685	467.045	651.920	–113.507
350	438.051	666.739	606.891	20.947	461.584	683.177	–101.956
400	499.642	729.313	618.285	44.411	456.833	715.155	–93.388
450	555.524	791.447	634.080	70.815	452.709	747.698	–86.789
500	605.529	852.616	652.885	99.866	449.123	780.693	–81.557
600	689.426	970.737	696.103	164.780	443.266	847.587	–73.788
700	755.715	1082.186	743.380	237.164	438.956	915.342	–68.302
800	808.765	1186.688	792.334	315.483	436.021	983.602	–64.221
900	851.879	1284.520	841.646	398.587	434.283	1052.149	–61.064
1000	887.396	1376.172	890.565	485.607	433.580	1120.847	–58.546
1100	916.979	1462.179	938.661	575.869	433.711	1189.584	–56.487
1200	941.838	1543.063	985.692	668.845	434.533	1258.258	–54.769
1300	962.887	1619.304	1031.527	764.110	435.860	1326.854	–53.313
1400	980.827	1691.336	1076.108	861.319	437.557	1395.337	–52.060
1500	996.211	1759.544	1119.417	960.190	439.544	1463.691	–50.969
1600	1009.475	1824.271	1161.465	1060.491	441.686	1531.895	–50.010
1700	1020.972	1885.823	1202.278	1162.027	443.910	1599.938	–49.159
1800	1030.988	1944.471	1241.895	1264.636	446.137	1667.919	–48.401
1900	1039.755	2000.453	1280.357	1368.183	448.338	1735.719	–47.717
2000	1047.463	2053.986	1317.710	1472.552	450.457	1803.433	–47.100
2100	1054.269	2105.260	1354.000	1577.645	452.413	1871.030	–46.538
2200	1060.304	2154.447	1389.274	1683.380	454.205	1938.540	–46.026
2300	1065.675	2201.700	1423.576	1789.684	455.831	2005.972	–45.556
2400	1070.474	2247.158	1456.951	1896.496	457.215	2073.285	–45.123
2500	1074.776	2290.945	1489.441	2003.762	458.372	2140.668	–44.726
2600	1078.647	2333.176	1521.085	2111.437	459.262	2207.883	–44.356
2700	1082.139	2373.951	1551.921	2219.479	459.892	2275.149	–44.014
2800	1085.300	2413.364	1581.987	2327.853	460.235	2342.418	–43.697
2900	1088.170	2451.499	1611.317	2436.529	460.259	2409.624	–43.401
3000	1090.781	2488.434	1639.942	2545.479	460.012	2476.863	–43.125
3100	1093.165	2524.240	1667.893	2654.678	459.411	2544.030	–42.866
3200	1095.345	2558.982	1695.199	2764.105	458.503	2611.303	–42.624
3300	1097.345	2592.719	1721.888	2873.741	457.266	2678.653	–42.399
3400	1099.182	2625.505	1747.985	2983.568	455.672	2745.949	–42.185
3500	1100.875	2657.393	1773.515	3093.573	453.726	2813.277	–41.985
3600	1102.437	2688.427	1798.500	3203.739	451.453	2880.764	–41.798
3700	1103.882	2718.653	1822.962	3314.056	448.818	2948.334	–41.622
3800	1105.220	2748.110	1846.922	3424.512	445.793	3015.918	–41.456
3900	1106.462	2776.834	1870.399	3535.097	442.424	3083.526	–41.298
4000	1107.617	2804.862	1893.412	3645.801	438.693	3151.380	–41.152
4100	1108.692	2832.226	1915.977	3756.617	434.561	3219.250	–41.013
4200	1109.695	2858.955	1938.112	3867.537	430.059	3287.216	–40.882
4300	1110.632	2885.077	1959.832	3978.554	425.172	3355.195	–40.757
4400	1111.508	2910.620	1981.152	4089.662	419.909	3423.392	–40.640
4500	1112.329	2935.608	2002.085	4200.854	414.288	3491.773	–40.531
4600	1113.099	2960.065	2022.646	4312.126	408.249	3560.295	–40.428
4700	1113.822	2984.011	2042.847	4423.472	401.812	3628.827	–40.329
4800	1114.502	3007.468	2062.700	4534.889	395.024	3697.616	–40.237
4900	1115.143	3030.455	2082.216	4646.371	387.807	3766.401	–40.150
5000	1115.746	3052.990	2101.407	4757.916	380.262	3835.542	–40.069

3.390. Phenanthro[9,10,1,2,3-*pqrst*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-79-2
Point Group: C_s

Length: 15.89 Å
Width: 12.90 Å
Breadth: 3.887 Å
L/B Ratio: 1.232

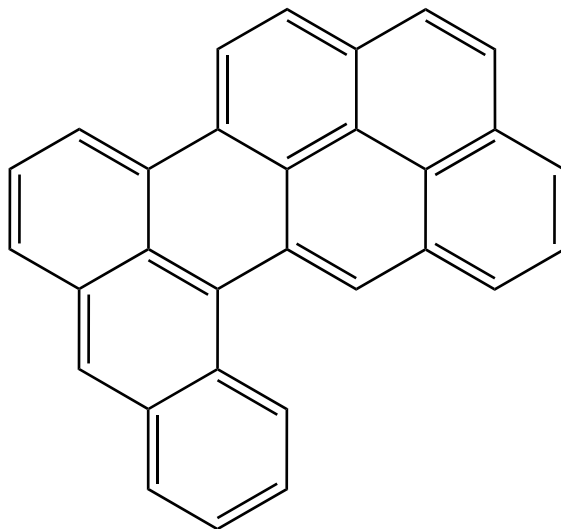
Cartesian coordinates:

C	4.8829	-2.5003	0.0000	C	-2.5790	2.2357	0.0000	H	6.3303	0.5885	0.0000
C	5.8888	-1.5144	0.0000	C	-3.9295	2.6454	0.0000	H	2.7606	-2.8950	0.0000
C	5.5522	-0.1834	0.0000	C	-4.9373	1.7070	0.0000	H	4.6442	2.3419	0.0000
C	3.5589	-2.1369	0.0000	C	-4.6348	0.3394	0.0000	H	2.9656	4.1246	0.0000
C	3.1853	-0.7722	0.0000	C	-0.9012	0.4422	0.0000	H	0.5933	4.8326	0.0000
C	4.1920	0.2121	0.0000	C	-2.2697	0.8590	0.0000	H	-1.7865	4.2632	0.0000
C	3.8404	1.5952	0.0000	C	-3.3184	-0.0981	0.0000	H	1.0264	-2.3977	0.0000
C	2.5275	1.9839	0.0000	C	-0.5670	-0.9453	0.0000	H	-4.1651	3.7157	0.0000
C	2.1553	3.3862	0.0000	C	-1.6418	-1.9320	0.0000	H	-5.9856	2.0236	0.0000
C	0.8663	3.7708	0.0000	C	-2.9854	-1.5183	0.0000	H	-5.4477	-0.4030	0.0000
C	-0.2138	2.8021	0.0000	C	-4.0004	-2.4877	0.0000	H	-5.0496	-2.1540	0.0000
C	-1.5246	3.1978	0.0000	C	-3.6938	-3.8368	0.0000	H	-4.4956	-4.5823	0.0000
C	1.4826	0.9973	0.0000	C	-2.3601	-4.2475	0.0000	H	-2.1166	-5.3149	0.0000
C	0.1201	1.4035	0.0000	C	-1.3479	-3.3045	0.0000	H	-0.2926	-3.6188	0.0000
C	0.7586	-1.3235	0.0000	H	5.1670	-3.5576	0.0000				
C	1.8026	-0.3689	0.0000	H	6.9399	-1.8207	0.0000				

Table 3.390: Table of thermodynamic data as a function of temperature for Phenanthro[9,10,1,2,3-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} [°]	<i>S</i> [°]	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> [°] (<i>T</i>) - <i>H</i> [°] (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.735	466.815	466.815	∞
100	115.392	359.836	826.890	-46.705	493.584	541.038	-282.603
200	233.781	474.230	621.859	-29.526	479.432	594.137	-155.169
250	301.976	533.672	598.244	-16.143	472.766	623.583	-130.288
298.15	368.392	592.553	592.553	0.000	466.815	653.185	-114.433
300	370.914	594.839	592.560	0.684	466.595	654.340	-113.928
350	437.264	657.048	597.321	20.904	461.094	686.078	-102.389
400	498.894	719.520	608.693	44.331	456.304	718.544	-93.830
450	554.810	781.568	624.461	70.698	452.144	751.578	-87.239
500	604.849	842.663	643.236	99.714	448.523	785.070	-82.014
600	688.816	960.666	686.393	164.564	442.601	852.965	-74.256
700	755.175	1072.027	733.612	236.890	438.234	921.732	-68.779
800	808.290	1176.461	782.512	315.159	435.248	991.011	-64.705
900	851.461	1274.241	831.776	398.218	433.466	1060.583	-61.553
1000	887.028	1365.851	880.652	485.198	432.724	1130.311	-59.040
1100	916.652	1451.825	928.710	575.426	432.820	1200.082	-56.986
1200	941.548	1532.682	975.706	668.371	433.611	1269.793	-55.271
1300	962.628	1608.901	1021.510	763.609	434.910	1339.428	-53.818
1400	980.595	1680.915	1066.062	860.793	436.583	1408.952	-52.568
1500	996.002	1749.107	1109.346	959.643	438.548	1478.349	-51.480
1600	1009.286	1813.822	1151.370	1059.923	440.671	1547.598	-50.523
1700	1020.801	1875.364	1192.163	1161.441	442.876	1616.686	-49.674
1800	1030.832	1934.001	1231.760	1264.034	445.087	1685.713	-48.917
1900	1039.612	1989.976	1270.205	1367.566	447.273	1754.561	-48.235
2000	1047.332	2043.502	1307.541	1471.921	449.379	1823.323	-47.619
2100	1054.149	2094.769	1343.816	1577.002	451.322	1891.969	-47.059
2200	1060.193	2143.951	1379.076	1682.725	453.103	1960.528	-46.548
2300	1065.573	2191.199	1413.365	1789.018	454.718	2029.010	-46.079
2400	1070.379	2236.653	1446.728	1895.820	456.092	2097.373	-45.647
2500	1074.688	2280.437	1479.206	2003.078	457.239	2165.807	-45.251
2600	1078.564	2322.664	1510.839	2110.744	458.121	2234.073	-44.882
2700	1082.062	2363.436	1541.666	2218.778	458.743	2302.390	-44.542
2800	1085.228	2402.846	1571.723	2327.145	459.078	2370.711	-44.225
2900	1088.102	2440.979	1601.043	2435.814	459.095	2438.969	-43.930
3000	1090.718	2477.912	1629.660	2544.757	458.842	2507.260	-43.654
3100	1093.105	2513.716	1657.603	2653.950	458.235	2575.479	-43.396
3200	1095.289	2548.456	1684.902	2763.371	457.320	2643.805	-43.155
3300	1097.292	2582.191	1711.584	2873.001	456.079	2712.208	-42.930
3400	1099.132	2614.976	1737.675	2982.824	454.479	2780.556	-42.717
3500	1100.827	2646.862	1763.198	3092.823	452.529	2848.938	-42.517
3600	1102.392	2677.895	1788.177	3202.985	450.250	2917.477	-42.331
3700	1103.839	2708.120	1812.634	3313.297	447.611	2986.101	-42.155
3800	1105.179	2737.575	1836.588	3423.749	444.583	3054.738	-41.989
3900	1106.423	2766.299	1860.060	3534.330	441.210	3123.400	-41.832
4000	1107.580	2794.326	1883.068	3645.031	437.474	3192.307	-41.686
4100	1108.657	2821.688	1905.629	3755.843	433.339	3261.231	-41.548
4200	1109.661	2848.416	1927.759	3866.760	428.833	3330.251	-41.417
4300	1110.600	2874.538	1949.475	3977.773	423.943	3399.283	-41.292
4400	1111.477	2900.081	1970.790	4088.878	418.677	3468.534	-41.176
4500	1112.300	2925.068	1991.720	4200.067	413.052	3537.969	-41.067
4600	1113.071	2949.524	2012.277	4311.336	407.011	3607.545	-40.964
4700	1113.795	2973.469	2032.474	4422.680	400.571	3677.131	-40.866
4800	1114.476	2996.926	2052.323	4534.094	393.781	3746.975	-40.775
4900	1115.118	3019.912	2071.836	4645.574	386.561	3816.815	-40.687
5000	1115.722	3042.447	2091.024	4757.116	379.013	3887.009	-40.606

3.391. Benzo[*a*]naphtho[2,1,8-*lmn*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-71-4
Point Group: C₁

Length: 14.38 Å
Width: 11.74 Å
Breadth: 5.189 Å
L/B Ratio: 1.225

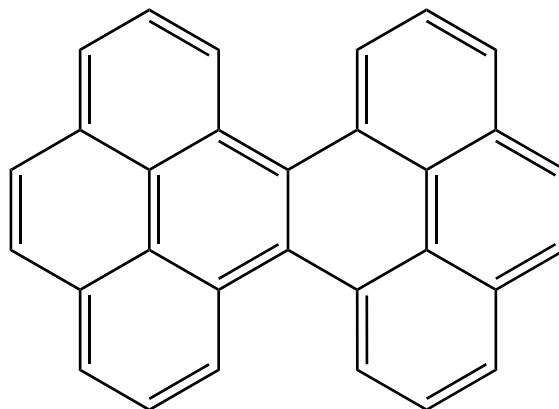
Cartesian coordinates:

C	4.1391	2.9325	-0.6496	C	-1.4427	0.2892	-0.0225	H	2.1640	3.7381	-0.9787
C	4.9020	1.8212	-0.3101	C	-4.2459	0.0002	-0.2899	H	6.1273	-0.4888	0.3708
C	2.7529	2.8540	-0.7095	C	-2.2956	1.4002	0.1860	H	4.9953	-2.6656	0.7542
C	4.2806	0.5998	-0.0321	C	-3.7007	1.2491	0.0041	H	2.9412	-4.0206	0.7723
C	5.0374	-0.5796	0.3003	C	-4.5687	2.3827	0.1387	H	0.4771	-4.1971	0.4549
C	4.4198	-1.7653	0.5097	C	-4.0789	3.5928	0.5149	H	0.1116	2.4620	-0.6688
C	2.9881	-1.8869	0.4135	C	-2.6910	3.7354	0.7898	H	-5.3241	-0.0996	-0.4678
C	2.3489	-3.1243	0.5565	C	-1.8404	2.6860	0.6284	H	-5.6383	2.2438	-0.0572
C	0.9776	-3.2179	0.3985	C	-3.4295	-1.1308	-0.3173	H	-4.7359	4.4614	0.6252
C	2.8718	0.5120	-0.0909	C	-2.0249	-0.9922	-0.1507	H	-2.3204	4.7039	1.1418
C	2.2141	-0.7358	0.1484	C	-1.2372	-2.1939	-0.0877	H	-0.7742	2.8184	0.8591
C	0.6709	1.5454	-0.4297	C	-1.8315	-3.4228	-0.2332	H	-1.2180	-4.3342	-0.1600
C	2.1034	1.6480	-0.4235	C	-3.2242	-3.5411	-0.4638	H	-3.6555	-4.5382	-0.5993
C	0.8031	-0.8188	0.0764	C	-4.0053	-2.4272	-0.5039	H	-5.0862	-2.5002	-0.6696
C	0.1972	-2.0813	0.1469	H	4.6369	3.8822	-0.8726				
C	0.0193	0.3867	-0.1177	H	5.9941	1.8975	-0.2627				

Table 3.391: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[2,1,8-*lmn*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.434	513.243	513.243	∞
100	113.185	353.440	819.804	-46.636	540.081	588.174	-307.224
200	233.580	466.908	614.801	-29.578	525.807	641.976	-167.664
250	302.568	526.396	591.135	-16.185	519.152	671.788	-140.360
298.15	369.504	585.428	585.428	0.000	513.243	701.737	-122.939
300	372.041	587.722	585.435	0.686	513.025	702.905	-122.384
350	438.721	650.131	590.212	20.972	507.589	734.994	-109.690
400	500.531	712.811	601.620	44.476	502.877	767.800	-100.262
450	556.524	775.057	617.440	70.928	498.801	801.165	-92.995
500	606.573	836.334	636.275	100.029	495.267	834.978	-87.228
600	690.447	954.644	679.564	165.048	489.513	903.490	-78.654
700	756.656	1066.246	726.916	237.530	485.302	972.846	-72.593
800	809.613	1170.867	775.943	315.939	482.456	1042.694	-68.080
900	852.638	1268.794	825.324	399.123	480.798	1112.818	-64.585
1000	888.075	1360.521	874.307	486.214	480.167	1183.085	-61.797
1100	917.586	1446.589	922.461	576.541	480.362	1253.384	-59.517
1200	942.383	1527.523	969.545	669.575	481.242	1323.614	-57.614
1300	963.377	1603.806	1015.428	764.891	482.620	1393.762	-56.001
1400	981.270	1675.872	1060.053	862.147	484.364	1463.793	-54.614
1500	996.611	1744.109	1103.402	961.060	486.393	1533.692	-53.407
1600	1009.839	1808.862	1145.487	1061.399	488.574	1603.439	-52.346
1700	1021.304	1870.435	1186.335	1162.969	490.833	1673.021	-51.405
1800	1031.292	1929.100	1225.983	1265.610	493.092	1742.540	-50.566
1900	1040.033	1985.099	1264.474	1369.186	495.321	1811.876	-49.811
2000	1047.719	2038.645	1301.854	1473.582	497.467	1881.125	-49.129
2100	1054.505	2089.931	1338.169	1578.700	499.447	1950.256	-48.509
2200	1060.522	2139.128	1373.466	1684.457	501.262	2019.298	-47.943
2300	1065.878	2186.391	1407.790	1790.782	502.910	2088.261	-47.425
2400	1070.662	2231.857	1441.184	1897.614	504.313	2157.104	-46.947
2500	1074.951	2275.652	1473.693	2004.898	505.488	2226.018	-46.509
2600	1078.810	2317.889	1505.354	2112.590	506.395	2294.761	-46.101
2700	1082.292	2358.670	1536.208	2220.648	507.041	2363.556	-45.725
2800	1085.443	2398.088	1566.289	2329.037	507.398	2432.353	-45.375
2900	1088.304	2436.228	1595.633	2437.727	507.436	2501.086	-45.048
3000	1090.907	2473.168	1624.272	2546.689	507.202	2569.852	-44.744
3100	1093.284	2508.978	1652.236	2655.901	506.614	2638.545	-44.458
3200	1095.457	2543.723	1679.555	2765.339	505.716	2707.344	-44.192
3300	1097.451	2577.463	1706.255	2874.986	504.491	2776.220	-43.943
3400	1099.283	2610.253	1732.364	2984.824	502.907	2845.041	-43.708
3500	1100.970	2642.143	1757.904	3094.838	500.971	2913.894	-43.487
3600	1102.527	2673.181	1782.899	3205.014	498.707	2982.906	-43.280
3700	1103.967	2703.409	1807.371	3315.339	496.080	3052.001	-43.086
3800	1105.301	2732.867	1831.340	3425.803	493.065	3121.109	-42.902
3900	1106.539	2761.594	1854.826	3536.396	489.703	3190.241	-42.728
4000	1107.690	2789.624	1877.847	3647.108	485.980	3259.619	-42.565
4100	1108.762	2816.989	1900.421	3757.932	481.855	3329.012	-42.411
4200	1109.762	2843.720	1922.563	3868.858	477.360	3398.502	-42.266
4300	1110.696	2869.844	1944.290	3979.882	472.479	3468.004	-42.127
4400	1111.570	2895.389	1965.617	4090.996	467.223	3537.724	-41.997
4500	1112.388	2920.378	1986.557	4202.194	461.607	3607.628	-41.875
4600	1113.156	2944.836	2007.125	4313.472	455.575	3677.674	-41.760
4700	1113.877	2968.783	2027.331	4424.824	449.143	3747.728	-41.650
4800	1114.555	2992.241	2047.190	4536.245	442.361	3818.040	-41.548
4900	1115.193	3015.229	2066.712	4647.733	435.148	3888.348	-41.449
5000	1115.794	3037.765	2085.909	4759.283	427.608	3959.011	-41.359

3.392. Tetrabenzo[*de,hi,mn,qr*]naphthacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 385-13-7
Point Group: C_{2h}

Length: 14.07 Å
Width: 11.43 Å
Breadth: 4.812 Å
L/B Ratio: 1.231

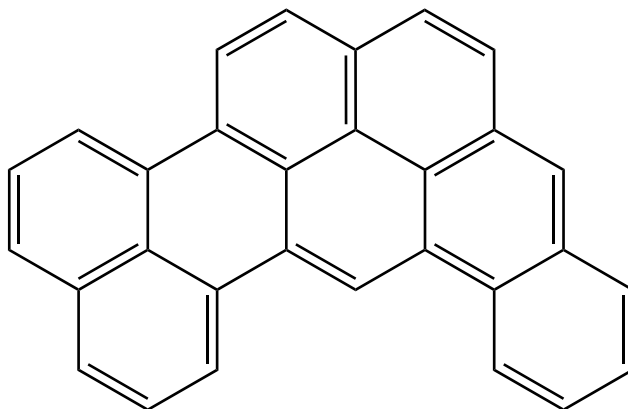
Cartesian coordinates:

C	-3.7395	-2.7879	0.1080	C	1.2615	-1.4173	-0.1409	H	-2.6023	-4.5097	0.7181
C	-1.3577	-2.7684	0.4870	C	3.7396	-2.7879	-0.1080	H	-5.8426	-1.2435	-0.5341
C	-2.5733	-3.4454	0.4609	C	2.5734	-3.4454	-0.4609	H	-5.8424	1.2455	-0.5306
C	-3.7058	-1.4084	-0.1230	C	1.3578	-2.7685	-0.4869	H	-4.6887	3.3307	0.0547
C	-4.9204	-0.6750	-0.3684	C	1.2611	1.4168	-0.1425	H	-2.6004	4.5088	0.7251
C	-4.9203	0.6764	-0.3667	C	1.3565	2.7676	-0.4903	H	-0.4587	3.3269	0.7862
C	-3.7055	1.4090	-0.1196	C	2.5720	3.4449	-0.4666	H	4.6897	-3.3298	-0.0461
C	-3.7388	2.7879	0.1144	C	3.7388	2.7880	-0.1144	H	2.6023	-4.5097	-0.7181
C	-2.5720	3.4448	0.4666	C	2.4761	-0.7155	0.0570	H	0.4608	-3.3286	-0.7839
C	-1.3566	2.7676	0.4903	C	2.4759	0.7156	0.0557	H	0.4588	3.3271	-0.7862
C	-2.4761	-0.7155	-0.0570	C	3.7055	1.4090	0.1196	H	2.6004	4.5088	-0.7251
C	-2.4759	0.7156	-0.0557	C	4.9203	0.6764	0.3667	H	4.6887	3.3307	-0.0547
C	-1.2611	1.4168	0.1425	C	4.9204	-0.6749	0.3684	H	5.8424	1.2455	0.5306
C	-1.2615	-1.4173	0.1409	C	3.7058	-1.4084	0.1229	H	5.8426	-1.2435	0.5341
C	0.0000	-0.6935	0.0000	H	-4.6896	-3.3300	0.0462				
C	-0.0000	0.6928	0.0000	H	-0.4610	-3.3290	0.7840				

Table 3.392: Table of thermodynamic data as a function of temperature for Tetra-benzo[de,hi,mn,qr]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.071	523.722	523.722	∞
100	111.296	345.919	809.746	-46.383	550.813	599.659	-313.223
200	232.329	458.268	605.680	-29.482	536.382	654.279	-170.877
250	301.593	517.506	582.084	-16.144	529.672	684.530	-143.022
298.15	368.797	576.390	576.390	0.000	523.722	714.911	-125.247
300	371.345	578.679	576.397	0.685	523.503	716.095	-124.681
350	438.295	641.002	581.166	20.943	518.039	748.639	-111.726
400	500.337	703.640	592.561	44.432	513.312	781.903	-102.104
450	556.510	765.874	608.367	70.878	509.230	815.727	-94.685
500	606.686	827.157	627.192	99.982	505.698	849.998	-88.797
600	690.691	945.502	670.468	165.020	499.964	919.427	-80.042
700	756.922	1057.143	717.817	237.529	495.779	989.695	-73.850
800	809.852	1161.798	766.845	315.963	492.959	1060.451	-69.239
900	852.832	1259.751	816.231	399.169	491.323	1131.481	-65.668
1000	888.222	1351.496	865.219	486.277	490.709	1202.650	-62.819
1100	917.692	1437.577	913.380	576.616	490.916	1273.851	-60.489
1200	942.455	1518.518	960.470	669.659	491.805	1344.982	-58.544
1300	963.422	1594.806	1006.359	764.981	493.189	1416.030	-56.896
1400	981.294	1666.874	1050.989	862.240	494.936	1486.961	-55.478
1500	996.620	1735.113	1094.343	961.155	496.967	1557.760	-54.245
1600	1009.836	1799.865	1136.432	1061.494	499.148	1628.407	-53.161
1700	1021.292	1861.438	1177.283	1163.064	501.406	1698.889	-52.199
1800	1031.274	1920.102	1216.934	1265.703	503.663	1769.307	-51.343
1900	1040.011	1976.100	1255.428	1369.277	505.891	1839.543	-50.572
2000	1047.693	2029.645	1292.810	1473.670	508.034	1909.693	-49.875
2100	1054.478	2080.929	1329.127	1578.786	510.012	1979.723	-49.242
2200	1060.493	2130.125	1364.425	1684.540	511.824	2049.665	-48.664
2300	1065.848	2177.387	1398.751	1790.862	513.468	2119.529	-48.135
2400	1070.632	2222.852	1432.147	1897.691	514.869	2189.273	-47.647
2500	1074.922	2266.645	1464.657	2004.972	516.040	2259.087	-47.200
2600	1078.781	2308.881	1496.319	2112.661	516.945	2328.731	-46.784
2700	1082.263	2349.661	1527.174	2220.716	517.588	2398.426	-46.399
2800	1085.415	2389.078	1557.256	2329.102	517.942	2468.124	-46.042
2900	1088.277	2427.218	1586.601	2437.789	517.977	2537.758	-45.709
3000	1090.881	2464.157	1615.240	2546.749	517.741	2607.425	-45.398
3100	1093.258	2499.966	1643.205	2655.958	517.150	2677.020	-45.107
3200	1095.433	2534.710	1670.524	2765.394	516.250	2746.720	-44.835
3300	1097.427	2568.449	1697.226	2875.038	515.022	2816.497	-44.581
3400	1099.259	2601.238	1723.334	2984.874	513.436	2886.220	-44.340
3500	1100.948	2633.128	1748.875	3094.885	511.497	2955.975	-44.115
3600	1102.506	2664.165	1773.870	3205.059	509.231	3025.888	-43.904
3700	1103.946	2694.392	1798.343	3315.383	506.603	3095.884	-43.705
3800	1105.281	2723.850	1822.312	3425.845	503.585	3165.894	-43.517
3900	1106.520	2752.577	1845.798	3536.436	500.222	3235.928	-43.340
4000	1107.672	2780.606	1868.820	3647.146	496.496	3306.207	-43.174
4100	1108.744	2807.971	1891.393	3757.967	492.369	3376.503	-43.016
4200	1109.745	2834.701	1913.536	3868.892	487.872	3446.894	-42.868
4300	1110.679	2860.825	1935.263	3979.914	482.990	3517.298	-42.726
4400	1111.554	2886.369	1956.590	4091.026	477.732	3587.921	-42.593
4500	1112.372	2911.358	1977.531	4202.223	472.115	3658.727	-42.469
4600	1113.141	2935.815	1998.098	4313.499	466.081	3729.674	-42.351
4700	1113.862	2959.763	2018.305	4424.850	459.648	3800.631	-42.238
4800	1114.540	2983.220	2038.164	4536.270	452.864	3871.845	-42.133
4900	1115.179	3006.208	2057.686	4647.756	445.650	3943.055	-42.033
5000	1115.781	3028.744	2076.883	4759.305	438.109	4014.620	-41.940

3.393. Anthra[9,1,2-*bcd*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120864-21-3
Point Group: C_s

Length: 15.37 Å
Width: 11.63 Å
Breadth: 3.886 Å
L/B Ratio: 1.322

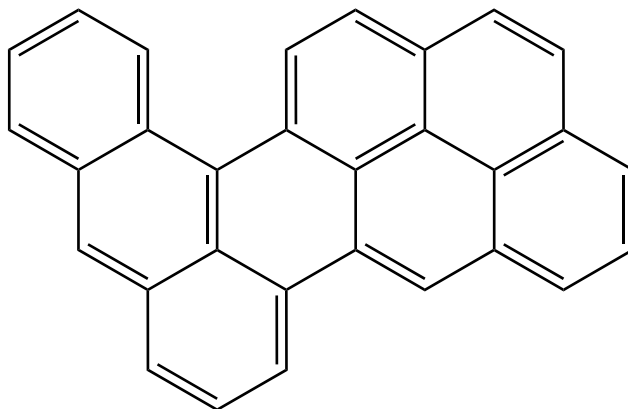
Cartesian coordinates:

C	-3.0037	-3.5264	0.0000	C	1.8286	-0.4660	0.0000	H	-5.1511	-3.4754	0.0000
C	-1.8123	-2.7737	0.0000	C	4.1886	1.0854	0.0000	H	-4.4797	2.4142	0.0000
C	-4.2199	-2.8977	0.0000	C	1.7628	0.9317	0.0000	H	-6.5690	1.0693	0.0000
C	-4.2914	-1.4790	0.0000	C	2.9632	1.7110	0.0000	H	-6.4639	-1.4163	0.0000
C	-4.4194	1.3149	0.0000	C	2.8547	3.1539	0.0000	H	-0.8729	4.7280	0.0000
C	-5.6037	0.5523	0.0000	C	1.6528	3.7652	0.0000	H	-2.9648	3.3855	0.0000
C	-5.5469	-0.8162	0.0000	C	0.4250	3.0031	0.0000	H	0.6872	-2.3220	0.0000
C	-3.1014	-0.7200	0.0000	C	0.4897	1.5874	0.0000	H	5.1134	1.6756	0.0000
C	-1.8438	-1.3943	0.0000	C	4.2784	-0.3311	0.0000	H	3.7844	3.7348	0.0000
C	-3.1816	0.7046	0.0000	C	3.1055	-1.1146	0.0000	H	1.5743	4.8586	0.0000
C	-1.9485	1.4878	0.0000	C	3.2243	-2.5290	0.0000	H	2.2995	-3.1263	0.0000
C	-0.8158	3.6335	0.0000	C	4.4559	-3.1275	0.0000	H	4.5433	-4.2188	0.0000
C	-1.9861	2.8806	0.0000	C	5.6298	-2.3414	0.0000	H	6.6052	-2.8389	0.0000
C	-0.7001	0.8264	0.0000	C	5.5455	-0.9749	0.0000	H	6.4517	-0.3584	0.0000
C	-0.6107	-0.6095	0.0000	H	-2.9416	-4.6196	0.0000				
C	0.6157	-1.2170	0.0000	H	-0.8404	-3.2913	0.0000				

Table 3.393: Table of thermodynamic data as a function of temperature for Anthra[9,1,2-*bcd*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.916	481.135	481.135	∞
100	115.871	363.962	832.103	-46.814	507.795	554.836	-289.811
200	234.307	478.662	626.613	-29.590	493.687	607.505	-158.661
250	302.641	538.237	602.947	-16.178	487.051	636.727	-133.034
298.15	369.151	597.244	597.244	0.000	481.135	666.106	-116.697
300	371.675	599.535	597.251	0.685	480.916	667.252	-116.176
350	438.082	661.866	602.022	20.946	475.454	698.752	-104.281
400	499.735	724.449	613.415	44.414	470.706	730.974	-95.453
450	555.650	786.596	629.211	70.823	466.588	763.760	-88.653
500	605.670	847.779	648.019	99.880	463.009	796.997	-83.260
600	689.571	965.926	691.244	164.809	457.166	864.374	-75.249
700	755.850	1077.397	738.530	237.207	452.870	932.609	-69.591
800	808.885	1181.916	787.492	315.539	449.948	1001.346	-65.380
900	851.985	1279.762	836.812	398.654	448.221	1070.370	-62.121
1000	887.490	1371.423	885.740	485.684	447.528	1139.543	-59.522
1100	917.060	1457.439	933.843	575.955	447.668	1208.755	-57.398
1200	941.910	1538.329	980.881	668.939	448.497	1277.902	-55.624
1300	962.950	1614.576	1026.722	764.210	449.831	1346.971	-54.121
1400	980.884	1686.612	1071.308	861.425	451.534	1415.927	-52.828
1500	996.261	1754.824	1114.623	960.302	453.527	1484.753	-51.703
1600	1009.520	1819.555	1156.675	1060.607	455.674	1553.430	-50.713
1700	1021.013	1881.109	1197.493	1162.147	457.902	1621.944	-49.835
1800	1031.025	1939.759	1237.114	1264.760	460.133	1690.396	-49.053
1900	1039.788	1995.743	1275.580	1368.310	462.337	1758.667	-48.348
2000	1047.493	2049.278	1312.936	1472.683	464.459	1826.852	-47.712
2100	1054.297	2100.553	1349.230	1577.779	466.418	1894.920	-47.133
2200	1060.329	2149.741	1384.506	1683.516	468.213	1962.900	-46.604
2300	1065.699	2196.995	1418.811	1789.823	469.842	2030.803	-46.120
2400	1070.496	2242.454	1452.189	1896.637	471.228	2098.586	-45.674
2500	1074.796	2286.243	1484.680	2003.905	472.386	2166.440	-45.264
2600	1078.665	2328.474	1516.327	2111.582	473.279	2234.125	-44.883
2700	1082.156	2369.249	1547.166	2219.626	473.911	2301.861	-44.531
2800	1085.316	2408.663	1577.233	2328.002	474.255	2369.601	-44.205
2900	1088.185	2446.799	1606.565	2436.679	474.280	2437.276	-43.899
3000	1090.795	2483.735	1635.191	2545.630	474.035	2504.985	-43.615
3100	1093.178	2519.541	1663.144	2654.831	473.436	2572.622	-43.347
3200	1095.358	2554.283	1690.452	2764.259	472.528	2640.365	-43.099
3300	1097.356	2588.020	1717.142	2873.896	471.293	2708.185	-42.866
3400	1099.193	2620.807	1743.241	2983.725	469.700	2775.951	-42.646
3500	1100.885	2652.695	1768.772	3093.730	467.755	2843.749	-42.440
3600	1102.447	2683.730	1793.758	3203.898	465.483	2911.705	-42.247
3700	1103.891	2713.956	1818.222	3314.216	462.848	2979.746	-42.066
3800	1105.229	2743.412	1842.183	3424.673	459.825	3047.799	-41.894
3900	1106.470	2772.137	1865.661	3535.258	456.457	3115.877	-41.732
4000	1107.625	2800.166	1888.675	3645.964	452.726	3184.200	-41.581
4100	1108.700	2827.529	1911.241	3756.781	448.595	3252.540	-41.437
4200	1109.702	2854.258	1933.377	3867.701	444.094	3320.975	-41.302
4300	1110.639	2880.381	1955.098	3978.719	439.208	3389.424	-41.172
4400	1111.515	2905.924	1976.418	4089.827	433.946	3458.090	-41.052
4500	1112.335	2930.913	1997.353	4201.020	428.325	3526.941	-40.939
4600	1113.105	2955.369	2017.914	4312.292	422.287	3595.933	-40.832
4700	1113.828	2979.316	2038.116	4423.639	415.850	3664.934	-40.730
4800	1114.508	3002.773	2057.969	4535.057	409.063	3734.193	-40.635
4900	1115.148	3025.760	2077.486	4646.540	401.846	3803.448	-40.544
5000	1115.751	3048.295	2096.678	4758.085	394.302	3873.058	-40.461

3.394. Benzo[*a*]naphtho[8,1,2-*klm*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-73-6
Point Group: C₁

Length: 15.38 Å
Width: 11.43 Å
Breadth: 5.196 Å
L/B Ratio: 1.345

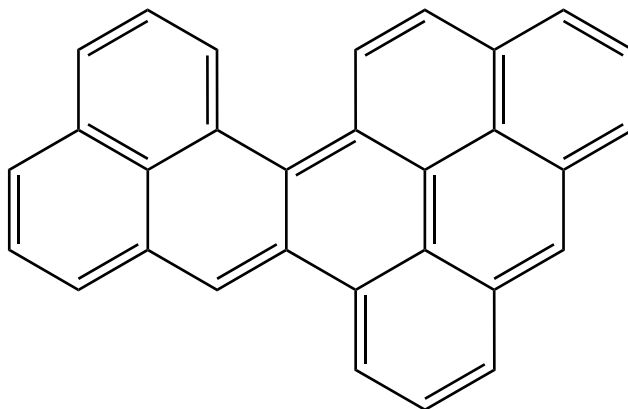
Cartesian coordinates:

C	-0.5000	-1.9721	0.1209	C	0.8502	2.9025	0.7131	H	-3.8846	-3.8862	0.4874
C	-0.5284	-3.3414	0.2128	C	2.0456	2.2316	0.4387	H	-5.1004	-1.8004	0.3122
C	-1.7512	-4.0421	0.3644	C	3.3150	2.9104	0.4493	H	-6.3527	0.2065	-0.0857
C	-2.9285	-3.3610	0.3817	C	4.4640	2.2446	0.1905	H	-6.4394	2.6184	-0.6987
C	-1.7274	0.1961	0.0825	C	4.4544	0.8309	-0.0860	H	-4.3306	3.8695	-1.0813
C	-1.7219	-1.2146	0.1598	C	5.6336	0.1273	-0.3493	H	-2.1490	2.8010	-0.7330
C	-2.9440	-1.9356	0.2482	C	5.5931	-1.2393	-0.6006	H	-1.2806	2.8020	0.8419
C	-4.1574	-1.2519	0.1941	C	4.3875	-1.9296	-0.5850	H	0.8749	3.9625	0.9910
C	-2.9594	0.8538	-0.1581	C	3.2207	0.1410	-0.0850	H	3.3211	3.9839	0.6700
C	-4.1761	0.1212	-0.0539	C	3.1923	-1.2511	-0.3236	H	5.4300	2.7624	0.1891
C	-5.4337	0.7878	-0.2242	C	1.9336	-1.9362	-0.2587	H	6.5920	0.6588	-0.3560
C	-5.4832	2.1033	-0.5621	C	0.7670	-1.2651	-0.0350	H	6.5231	-1.7788	-0.8093
C	-4.2743	2.8240	-0.7603	C	0.7583	0.1705	0.1154	H	4.3685	-3.0085	-0.7756
C	-3.0686	2.2243	-0.5633	C	1.9994	0.8493	0.1575	H	1.9226	-3.0333	-0.3631
C	-0.4461	0.8880	0.2581	H	0.4144	-3.9076	0.1583				
C	-0.3619	2.2393	0.6247	H	-1.7276	-5.1326	0.4587				

Table 3.394: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[8,1,2-*klm*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.625	516.573	516.573	∞
100	113.708	354.653	822.587	-46.793	543.254	591.226	-308.819
200	234.413	468.604	616.924	-29.664	529.051	644.882	-168.422
250	303.444	528.283	593.193	-16.228	522.440	674.604	-140.948
298.15	370.393	587.471	587.471	0.000	516.573	704.458	-123.416
300	372.931	589.770	587.478	0.688	516.357	705.622	-122.857
350	439.605	652.317	592.266	21.018	510.965	737.605	-110.079
400	501.393	715.113	603.698	44.566	506.297	770.299	-100.589
450	557.352	777.458	619.548	71.060	502.263	803.547	-93.271
500	607.358	838.821	638.417	100.202	498.769	837.237	-87.464
600	691.141	957.266	681.776	165.294	493.090	905.493	-78.829
700	757.260	1068.968	729.194	237.842	488.943	974.582	-72.723
800	810.138	1173.664	778.281	316.306	486.154	1044.153	-68.175
900	853.095	1271.649	827.716	399.540	484.545	1113.995	-64.653
1000	888.475	1363.421	876.748	486.673	483.957	1183.974	-61.843
1100	917.938	1449.525	924.945	577.038	484.189	1253.981	-59.545
1200	942.694	1530.488	972.068	670.104	485.102	1323.916	-57.627
1300	963.654	1606.794	1017.987	765.450	486.510	1393.766	-56.001
1400	981.517	1678.880	1062.643	862.732	488.279	1463.497	-54.603
1500	996.834	1747.133	1106.021	961.669	490.332	1533.094	-53.386
1600	1010.039	1811.899	1148.131	1062.029	492.534	1602.538	-52.316
1700	1021.486	1873.484	1189.003	1163.618	494.812	1671.817	-51.368
1800	1031.457	1932.159	1228.672	1266.277	497.088	1741.030	-50.522
1900	1040.184	1988.166	1267.183	1369.868	499.334	1810.059	-49.761
2000	1047.857	2041.720	1304.581	1474.278	501.494	1879.002	-49.073
2100	1054.632	2093.012	1340.912	1579.410	503.487	1947.824	-48.448
2200	1060.639	2142.215	1376.225	1685.179	505.314	2016.558	-47.878
2300	1065.986	2189.483	1410.563	1791.516	506.973	2085.213	-47.356
2400	1070.762	2234.953	1443.971	1898.357	508.387	2153.746	-46.874
2500	1075.044	2278.752	1476.492	2005.651	509.571	2222.350	-46.432
2600	1078.896	2320.993	1508.165	2113.352	510.487	2290.783	-46.021
2700	1082.373	2361.777	1539.030	2221.418	511.142	2359.267	-45.642
2800	1085.519	2401.198	1569.121	2329.815	511.507	2427.753	-45.289
2900	1088.375	2439.341	1598.475	2438.512	511.552	2496.175	-44.960
3000	1090.974	2476.283	1627.123	2547.482	511.325	2564.630	-44.653
3100	1093.346	2512.095	1655.095	2656.700	510.743	2633.011	-44.365
3200	1095.516	2546.842	1682.422	2766.144	509.852	2701.498	-44.097
3300	1097.506	2580.584	1709.131	2875.797	508.632	2770.062	-43.846
3400	1099.335	2613.375	1735.246	2985.640	507.053	2838.571	-43.608
3500	1101.020	2645.267	1760.793	3095.659	505.122	2907.112	-43.385
3600	1102.574	2676.306	1785.795	3205.840	502.863	2975.811	-43.177
3700	1104.012	2706.535	1810.273	3316.170	500.241	3044.594	-42.981
3800	1105.344	2735.995	1834.248	3426.639	497.230	3113.389	-42.796
3900	1106.580	2764.723	1857.740	3537.236	493.873	3182.209	-42.620
4000	1107.729	2792.754	1880.766	3647.952	490.153	3251.273	-42.456
4100	1108.799	2820.120	1903.345	3758.779	486.032	3320.354	-42.301
4200	1109.797	2846.851	1925.492	3869.709	481.540	3389.530	-42.154
4300	1110.730	2872.977	1947.224	3980.736	476.663	3458.719	-42.014
4400	1111.602	2898.522	1968.555	4091.853	471.410	3528.126	-41.883
4500	1112.419	2923.512	1989.500	4203.055	465.798	3597.717	-41.760
4600	1113.185	2947.970	2010.071	4314.335	459.768	3667.449	-41.644
4700	1113.905	2971.918	2030.282	4425.690	453.339	3737.190	-41.533
4800	1114.582	2995.377	2050.145	4537.115	446.560	3807.189	-41.430
4900	1115.219	3018.366	2069.671	4648.605	439.350	3877.183	-41.330
5000	1115.819	3040.902	2088.871	4760.157	431.812	3947.532	-41.239

3.395. Dibenzo[*de,mn*]naphtho[2,1,8-*gra*]naphthacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-68-9
Point Group: C₁

Length: 15.41 Å
Width: 11.45 Å
Breadth: 5.250 Å
L/B Ratio: 1.346

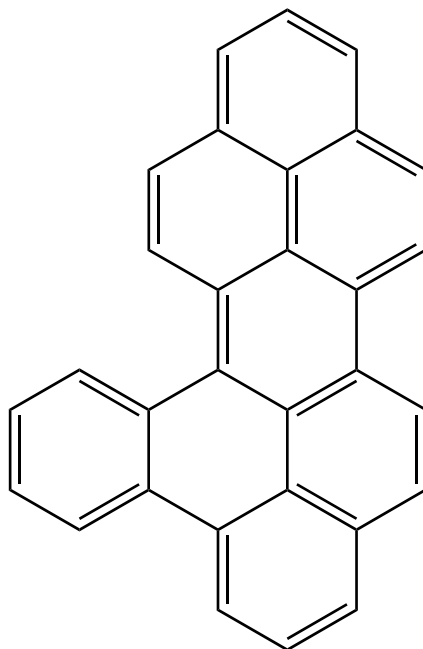
Cartesian coordinates:

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C	-4.0460	-1.4268	0.1407	C	4.5154	0.9678	0.0470	H	6.6523	0.8569	-0.3231
C	-4.1142	-0.0393	-0.0322	C	4.4626	-1.7302	-0.7134	H	6.5912	-1.5219	-1.0403
C	-2.9188	0.7203	-0.1291	C	5.6728	-1.0122	-0.7307	H	4.4608	-2.7932	-0.9792
C	-1.6613	0.0852	-0.0447	C	5.7066	0.3034	-0.3424	H	2.0765	-2.9261	-0.3283
C	-1.6110	-1.3103	0.1098	C	-3.0165	2.1378	-0.3103	H	-1.8621	3.9631	-0.6333
C	-0.3515	-1.9902	0.1561	C	-1.7856	2.8884	-0.4302	H	0.3264	2.8933	-0.4155
C	0.8708	-1.2018	0.0256	C	-0.5870	2.2906	-0.3093	H	-6.2894	0.0337	-0.0306
C	0.7894	0.2555	0.1020	C	-5.3735	0.6304	-0.1093	H	-6.3977	2.4967	-0.3340
C	-0.4321	0.8671	-0.0688	C	-5.4319	1.9836	-0.2768	H	-4.3194	3.8333	-0.5206
C	2.0481	-1.8284	-0.2300	C	-4.2455	2.7489	-0.3812	H	-4.9710	-2.0114	0.2187
C	3.2872	-1.1020	-0.3489	C	-2.7261	-3.4888	0.3725	H	0.6535	-3.8746	0.3233
C	3.2846	0.2811	-0.0123	C	-1.5143	-4.1072	0.4184	H	-1.4430	-5.1928	0.5421
C	2.0621	0.9560	0.3039	C	-0.3167	-3.3551	0.3046	H	-3.6565	-4.0618	0.4560
C	2.1486	2.2330	0.8240	H	5.5029	2.8342	0.5728				
C	3.3848	2.9040	0.9334	H	1.2424	2.7636	1.1473				

Table 3.395: Table of thermodynamic data as a function of temperature for Dibenzo[*de,mn*]naphtho[2,1,8-*gra*]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.772	571.433	571.433	∞
100	113.816	355.445	824.717	-46.927	597.980	645.873	-337.363
200	235.154	469.663	618.441	-29.756	583.820	699.438	-182.671
250	304.401	529.532	594.637	-16.276	577.251	729.103	-152.335
298.15	371.446	588.898	588.898	0.000	571.433	758.893	-132.952
300	373.985	591.204	588.905	0.690	571.219	760.054	-132.334
350	440.677	653.915	593.706	21.073	565.881	791.961	-118.191
400	502.436	716.853	605.167	44.674	561.266	824.572	-107.676
450	558.344	779.318	621.054	71.219	557.282	857.729	-99.561
500	608.288	840.782	639.964	100.409	553.836	891.323	-93.114
600	691.939	959.386	683.406	165.588	548.243	959.376	-83.519
700	757.937	1071.201	730.902	238.209	544.170	1028.246	-76.727
800	810.710	1175.980	780.060	316.736	541.443	1097.590	-71.664
900	853.581	1274.028	829.559	400.022	539.887	1167.196	-67.741
1000	888.890	1365.847	878.646	487.201	539.344	1236.935	-64.610
1100	918.294	1451.988	926.894	577.604	539.615	1306.698	-62.049
1200	943.003	1532.980	974.060	670.704	540.561	1376.385	-59.911
1300	963.924	1609.309	1020.018	766.078	541.998	1445.985	-58.099
1400	981.755	1681.414	1064.710	863.386	543.793	1515.463	-56.541
1500	997.044	1749.682	1108.119	962.345	545.868	1584.807	-55.187
1600	1010.226	1814.461	1150.258	1062.724	548.089	1653.995	-53.996
1700	1021.653	1876.057	1191.156	1164.331	550.385	1723.016	-52.941
1800	1031.607	1934.741	1230.849	1267.006	552.677	1791.972	-52.001
1900	1040.320	1990.756	1269.381	1370.612	554.937	1860.743	-51.154
2000	1047.981	2044.316	1306.799	1475.035	557.110	1929.426	-50.390
2100	1054.745	2095.614	1343.148	1580.178	559.115	1997.989	-49.696
2200	1060.742	2144.822	1378.477	1685.958	560.953	2066.462	-49.063
2300	1066.080	2192.094	1412.831	1792.304	562.622	2134.856	-48.483
2400	1070.850	2237.569	1446.254	1899.155	564.045	2203.128	-47.949
2500	1075.125	2281.371	1478.788	2006.458	565.237	2271.470	-47.459
2600	1078.971	2323.614	1510.474	2114.166	566.161	2339.641	-47.003
2700	1082.442	2364.401	1541.350	2222.240	566.823	2407.863	-46.582
2800	1085.584	2403.825	1571.452	2330.644	567.195	2476.086	-46.191
2900	1088.435	2441.970	1600.816	2439.347	567.246	2544.245	-45.826
3000	1091.031	2478.914	1629.473	2548.322	567.025	2612.437	-45.486
3100	1093.399	2514.728	1657.455	2657.545	566.449	2680.555	-45.166
3200	1095.566	2549.477	1684.791	2766.995	565.562	2748.779	-44.868
3300	1097.553	2583.220	1711.507	2876.653	564.348	2817.080	-44.590
3400	1099.380	2616.013	1737.630	2986.501	562.774	2885.325	-44.327
3500	1101.062	2647.906	1763.185	3096.524	560.847	2953.602	-44.079
3600	1102.614	2678.946	1788.193	3206.709	558.592	3022.037	-43.848
3700	1104.050	2709.176	1812.678	3317.043	555.974	3090.556	-43.630
3800	1105.379	2738.637	1836.659	3427.515	552.966	3159.087	-43.424
3900	1106.614	2767.366	1860.157	3538.115	549.613	3227.642	-43.229
4000	1107.761	2795.397	1883.189	3648.835	545.896	3296.442	-43.046
4100	1108.830	2822.764	1905.773	3759.665	541.778	3365.259	-42.873
4200	1109.827	2849.496	1927.925	3870.598	537.290	3434.171	-42.709
4300	1110.758	2875.622	1949.662	3981.628	532.415	3503.095	-42.553
4400	1111.629	2901.168	1970.998	4092.748	527.165	3572.237	-42.407
4500	1112.444	2926.159	1991.947	4203.952	521.555	3641.564	-42.269
4600	1113.210	2950.618	2012.523	4315.235	515.528	3711.031	-42.139
4700	1113.928	2974.566	2032.738	4426.592	509.102	3780.507	-42.015
4800	1114.604	2998.025	2052.605	4538.019	502.325	3850.241	-41.898
4900	1115.241	3021.014	2072.134	4649.512	495.117	3919.970	-41.787
5000	1115.840	3043.551	2091.338	4761.066	487.581	3990.055	-41.683

3.396. Tribenzo[*a,cd,lm*]perylene



Formula: $C_{30}H_{16}$
Mass: 376.448 g/mol
CAS Number: 92411-20-6
Point Group: C_1

Length: 15.80 Å
Width: 11.60 Å
Breadth: 5.058 Å
L/B Ratio: 1.362

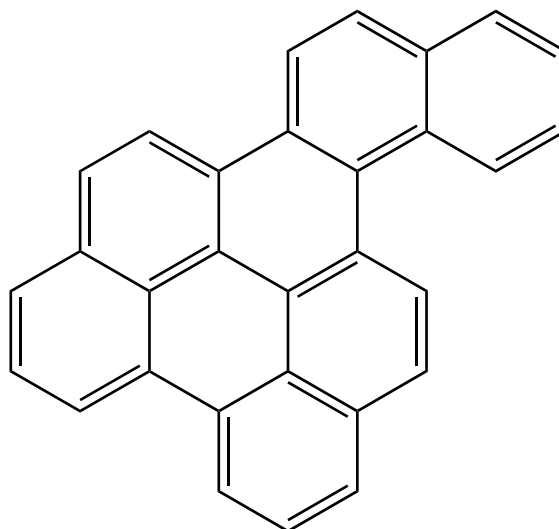
Cartesian coordinates:

C	-0.5118	-0.6199	-0.0354	C	-2.8450	2.3399	0.0978	H	-0.1059	-3.2171	-0.8291
C	-0.0837	1.8011	-0.1935	C	0.8681	-0.8364	0.1410	H	-1.7856	-5.0002	-0.9977
C	-0.9825	0.7213	-0.0764	C	2.7579	-2.3217	0.6302	H	-4.1716	-4.5412	-0.4400
C	-1.9078	3.4100	-0.0965	C	1.4281	-2.1113	0.5244	H	-4.8708	-2.2235	0.1445
C	-0.5905	3.1457	-0.2456	C	1.7779	0.2478	-0.0098	H	-5.3820	-0.5678	0.5737
C	-2.8711	-1.4131	0.0169	C	1.3081	1.5553	-0.2335	H	-6.1531	1.7914	0.7150
C	-1.5029	-1.6874	-0.1776	C	2.2537	2.6152	-0.4594	H	-4.5445	3.6553	0.3610
C	-1.1517	-2.9874	-0.5831	C	3.5876	2.3906	-0.4399	H	3.1514	-3.2985	0.9346
C	-2.0918	-3.9967	-0.6843	C	3.6981	-1.2672	0.3596	H	0.7352	-2.9327	0.7541
C	-3.4299	-3.7379	-0.3884	C	3.1947	0.0192	0.0594	H	1.8535	3.6226	-0.6502
C	-3.8126	-2.4530	-0.0551	C	4.1030	1.0776	-0.1676	H	4.3012	3.2020	-0.6232
C	-2.3880	1.0057	0.0612	C	5.4816	0.8344	-0.1176	H	6.1820	1.6568	-0.3022
C	-3.3243	-0.0439	0.2048	C	5.9585	-0.4369	0.1650	H	7.0380	-0.6181	0.2005
C	-4.6620	0.2555	0.4501	C	5.0757	-1.4846	0.4086	H	5.4598	-2.4842	0.6411
C	-5.0971	1.5783	0.5191	H	-2.2863	4.4383	-0.1169				
C	-4.2027	2.6146	0.3283	H	0.1355	3.9592	-0.3970				

Table 3.396: Table of thermodynamic data as a function of temperature for Tribenzo[*a,cd,lm*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.495	489.763	489.763	∞
100	113.657	354.765	821.246	-46.648	516.589	564.550	-294.885
200	233.639	468.452	616.257	-29.561	502.344	618.205	-161.455
250	302.374	527.924	592.609	-16.171	495.686	647.940	-135.377
298.15	369.131	586.906	586.906	0.000	489.763	677.816	-118.748
300	371.664	589.198	586.914	0.685	489.544	678.981	-118.219
350	438.242	651.541	591.685	20.949	484.087	710.998	-106.109
400	500.011	714.153	603.081	44.429	479.350	743.736	-97.120
450	555.999	776.337	618.884	70.854	475.247	777.035	-90.194
500	606.060	837.559	637.700	99.929	471.687	810.785	-84.700
600	689.976	955.780	680.948	164.899	465.884	879.180	-76.538
700	756.222	1067.311	728.260	237.336	461.627	948.426	-70.771
800	809.207	1171.876	777.248	315.702	458.740	1018.170	-66.478
900	852.255	1269.757	826.593	398.847	457.042	1088.195	-63.156
1000	887.712	1361.445	875.544	485.901	456.374	1158.368	-60.506
1100	917.242	1447.479	923.668	576.193	456.534	1228.576	-58.339
1200	942.059	1528.384	970.724	669.193	457.380	1298.719	-56.531
1300	963.072	1604.642	1016.582	764.478	458.727	1368.782	-54.997
1400	980.984	1676.686	1061.183	861.704	460.441	1438.730	-53.679
1500	996.344	1744.904	1104.511	960.590	462.443	1508.549	-52.531
1600	1009.589	1809.640	1146.576	1060.902	464.597	1578.217	-51.522
1700	1021.071	1871.198	1187.405	1162.449	466.832	1647.723	-50.627
1800	1031.074	1929.851	1227.036	1265.067	469.068	1717.166	-49.830
1900	1039.830	1985.838	1265.510	1368.622	471.277	1786.427	-49.111
2000	1047.528	2039.374	1302.875	1472.998	473.403	1855.603	-48.462
2100	1054.327	2090.651	1339.176	1578.098	475.365	1924.661	-47.872
2200	1060.355	2139.840	1374.459	1683.838	477.163	1993.631	-47.334
2300	1065.721	2187.095	1408.771	1790.147	478.794	2062.525	-46.840
2400	1070.516	2232.555	1442.154	1896.963	480.182	2131.297	-46.386
2500	1074.814	2276.345	1474.651	2004.233	481.342	2200.141	-45.968
2600	1078.681	2318.576	1506.303	2111.911	482.237	2268.816	-45.580
2700	1082.170	2359.352	1537.146	2219.957	482.870	2337.542	-45.222
2800	1085.328	2398.766	1567.218	2328.334	483.215	2406.271	-44.889
2900	1088.195	2436.903	1596.554	2437.013	483.242	2474.936	-44.577
3000	1090.805	2473.839	1625.184	2545.965	482.998	2543.635	-44.288
3100	1093.187	2509.646	1653.141	2655.166	482.399	2612.261	-44.015
3200	1095.366	2544.388	1680.452	2764.595	481.493	2680.993	-43.762
3300	1097.364	2578.125	1707.145	2874.233	480.258	2749.803	-43.525
3400	1099.200	2610.912	1733.247	2984.063	478.666	2818.558	-43.301
3500	1100.891	2642.800	1758.781	3094.069	476.722	2887.346	-43.090
3600	1102.452	2673.836	1783.770	3204.237	474.450	2956.292	-42.894
3700	1103.896	2704.062	1808.236	3314.555	471.816	3025.321	-42.709
3800	1105.233	2733.518	1832.199	3425.012	468.794	3094.364	-42.534
3900	1106.475	2762.244	1855.680	3535.599	465.426	3163.431	-42.369
4000	1107.629	2790.272	1878.696	3646.304	461.696	3232.744	-42.214
4100	1108.703	2817.636	1901.264	3757.122	457.565	3302.073	-42.068
4200	1109.706	2844.365	1923.402	3868.043	453.064	3371.498	-41.930
4300	1110.642	2870.488	1945.125	3979.061	448.178	3440.936	-41.798
4400	1111.518	2896.031	1966.447	4090.169	442.916	3510.592	-41.675
4500	1112.338	2921.019	1987.383	4201.362	437.295	3580.432	-41.560
4600	1113.108	2945.476	2007.946	4312.635	431.258	3650.413	-41.451
4700	1113.831	2969.422	2028.149	4423.982	424.821	3720.403	-41.347
4800	1114.510	2992.879	2048.005	4535.400	418.035	3790.652	-41.250
4900	1115.150	3015.866	2067.523	4646.883	410.818	3860.896	-41.157
5000	1115.753	3038.402	2086.716	4758.428	403.274	3931.495	-41.071

3.397. Phenanthro[1,2,3,4-ghi]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-58-7
Point Group: C₁

Length: 15.86 Å
Width: 11.65 Å
Breadth: 5.005 Å
L/B Ratio: 1.361

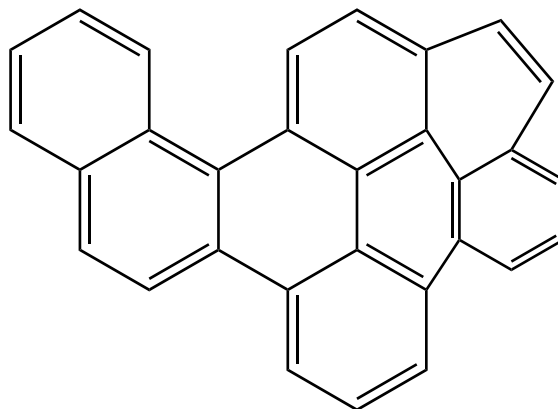
Cartesian coordinates:

C	-2.8944	-1.2242	0.0641	C	-0.8879	0.8210	-0.0574	H	-1.8691	-4.9702	-0.3227
C	-3.8481	-2.2302	0.1073	C	0.0835	1.8153	-0.1705	H	0.4658	-4.2971	-0.6508
C	-3.4819	-3.5758	-0.0241	C	-0.3253	3.1876	-0.1723	H	2.2064	-2.5701	-0.6174
C	-2.1619	-3.9205	-0.2075	C	-1.6294	3.5370	-0.0276	H	-4.2733	3.9503	0.3043
C	-0.5020	-0.5563	-0.1087	C	1.4715	1.4487	-0.2369	H	-6.0113	2.1829	0.5127
C	-1.5243	-1.5643	-0.0983	C	1.8676	0.1102	-0.1053	H	-5.3756	-0.2207	0.3987
C	-1.1695	-2.9189	-0.2481	C	3.7770	2.1823	-0.4545	H	0.4485	3.9615	-0.2856
C	0.2034	-3.2501	-0.4592	C	2.4533	2.4698	-0.4468	H	-1.9315	4.5906	-0.0155
C	1.1611	-2.2878	-0.4311	C	4.2201	0.8639	-0.1268	H	4.5245	2.9549	-0.6680
C	0.8510	-0.9108	-0.1879	C	3.2774	-0.1593	0.1056	H	2.1054	3.4987	-0.6235
C	-3.2765	0.1791	0.1654	C	3.7715	-1.3838	0.6187	H	3.0656	-2.1771	0.8996
C	-3.9969	2.8904	0.2705	C	5.1169	-1.6034	0.7911	H	5.4713	-2.5592	1.1912
C	-4.9585	1.9112	0.3829	C	6.0500	-0.6047	0.4636	H	7.1203	-0.8024	0.5802
C	-4.6010	0.5581	0.3245	C	5.6050	0.6162	0.0218	H	6.3156	1.4184	-0.2087
C	-2.6412	2.5357	0.1100	H	-4.9064	-1.9584	0.2434				
C	-2.2709	1.1767	0.0743	H	-4.2557	-4.3495	0.0156				

Table 3.397: Table of thermodynamic data as a function of temperature for Phenanthro[1,2,3,4-*ghi*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.567	483.407	483.407	∞
100	114.262	357.413	823.683	-46.627	510.254	557.951	-291.437
200	233.438	471.250	618.865	-29.523	496.026	611.328	-159.659
250	301.967	530.653	595.248	-16.149	489.353	640.924	-133.911
298.15	368.627	589.554	589.554	0.000	483.407	670.671	-117.496
300	371.157	591.842	589.561	0.684	483.188	671.831	-116.974
350	437.698	654.104	594.326	20.922	477.703	703.718	-105.022
400	499.462	716.643	605.708	44.374	472.939	736.329	-96.153
450	555.464	778.763	621.492	70.772	468.809	769.506	-89.320
500	605.547	839.930	640.287	99.821	465.223	803.136	-83.901
600	689.516	958.062	683.492	164.742	459.371	871.298	-75.852
700	755.813	1069.526	730.761	237.136	455.071	940.320	-70.166
800	808.843	1174.040	779.710	315.464	452.145	1009.845	-65.935
900	851.930	1271.880	829.020	398.574	450.414	1079.656	-62.660
1000	887.420	1363.535	877.938	485.597	449.715	1149.618	-60.049
1100	916.980	1449.543	926.033	575.861	449.846	1219.618	-57.914
1200	941.821	1530.427	973.063	668.836	450.668	1289.556	-56.132
1300	962.857	1606.666	1018.898	764.099	451.992	1359.415	-54.621
1400	980.788	1678.695	1063.478	861.304	453.686	1429.162	-53.322
1500	996.165	1746.900	1106.786	960.171	455.669	1498.781	-52.191
1600	1009.426	1811.625	1148.833	1060.467	457.806	1568.250	-51.197
1700	1020.921	1873.174	1189.646	1161.998	460.025	1637.558	-50.315
1800	1030.936	1931.818	1229.261	1264.602	462.247	1706.803	-49.529
1900	1039.703	1987.798	1267.722	1368.143	464.443	1775.869	-48.821
2000	1047.412	2041.328	1305.074	1472.507	466.557	1844.849	-48.182
2100	1054.219	2092.599	1341.363	1577.596	468.507	1913.712	-47.600
2200	1060.255	2141.784	1376.636	1683.325	470.295	1982.487	-47.069
2300	1065.628	2189.035	1410.937	1789.625	471.916	2051.186	-46.583
2400	1070.429	2234.491	1444.311	1896.432	473.295	2119.765	-46.135
2500	1074.733	2278.277	1476.799	2003.694	474.447	2188.416	-45.723
2600	1078.605	2320.505	1508.442	2111.364	475.333	2256.897	-45.341
2700	1082.099	2361.279	1539.278	2219.402	475.960	2325.431	-44.987
2800	1085.262	2400.690	1569.343	2327.773	476.298	2393.967	-44.659
2900	1088.133	2438.824	1598.671	2436.445	476.318	2462.440	-44.352
3000	1090.746	2475.758	1627.295	2545.391	476.068	2530.947	-44.067
3100	1093.131	2511.563	1655.245	2654.587	475.464	2599.381	-43.798
3200	1095.313	2546.304	1682.551	2764.010	474.552	2667.922	-43.548
3300	1097.314	2580.039	1709.239	2873.643	473.312	2736.540	-43.315
3400	1099.153	2612.825	1735.335	2983.468	471.715	2805.104	-43.094
3500	1100.847	2644.712	1760.863	3093.469	469.766	2873.700	-42.887
3600	1102.410	2675.746	1785.848	3203.633	467.490	2942.455	-42.693
3700	1103.856	2705.971	1810.309	3313.947	464.852	3011.294	-42.511
3800	1105.195	2735.427	1834.269	3424.400	461.826	3080.145	-42.339
3900	1106.438	2764.151	1857.745	3534.983	458.454	3149.022	-42.176
4000	1107.594	2792.178	1880.757	3645.685	454.720	3218.144	-42.024
4100	1108.670	2819.541	1903.322	3756.499	450.586	3287.282	-41.880
4200	1109.674	2846.269	1925.456	3867.417	446.082	3356.517	-41.744
4300	1110.611	2872.392	1947.175	3978.431	441.193	3425.764	-41.614
4400	1111.489	2897.934	1968.494	4089.537	435.928	3495.230	-41.493
4500	1112.310	2922.922	1989.427	4200.727	430.305	3564.880	-41.379
4600	1113.081	2947.378	2009.987	4311.997	424.265	3634.671	-41.272
4700	1113.805	2971.324	2030.187	4423.342	417.825	3704.471	-41.170
4800	1114.486	2994.780	2050.039	4534.757	411.036	3774.529	-41.074
4900	1115.127	3017.767	2069.555	4646.238	403.817	3844.583	-40.983
5000	1115.731	3040.302	2088.745	4757.781	396.270	3914.993	-40.899

3.398. Benzo[*pqr*]naphtho[1,2-*b*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-57-6
Point Group: C₁

Length: 15.88 Å
Width: 11.65 Å
Breadth: 5.032 Å
L/B Ratio: 1.363

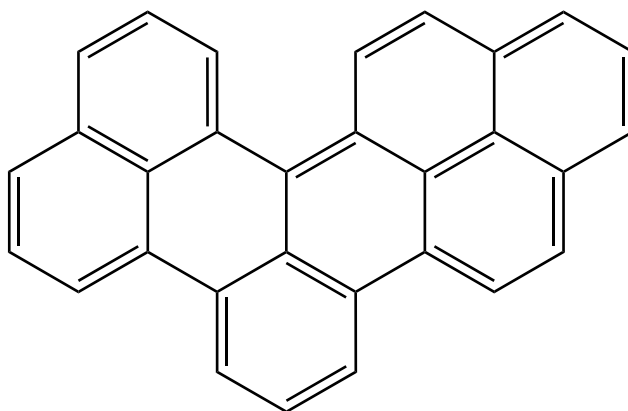
Cartesian coordinates:

C	5.9669	1.3705	0.4798	C	-2.0673	-3.1523	0.1342	H	2.7583	2.4421	0.8497
C	5.7355	0.0856	0.0636	C	-0.4883	0.2387	-0.1116	H	5.0650	3.2186	1.1589
C	3.5894	1.7700	0.5962	C	-0.6517	-1.1886	-0.0335	H	5.0598	-2.4142	-0.5813
C	4.8761	2.2101	0.7761	C	-1.9371	-1.7664	0.1040	H	2.7597	-3.3431	-0.5570
C	3.3080	0.4660	0.1114	C	-3.1116	-0.9080	0.1872	H	-0.1475	4.0645	-0.7600
C	4.4101	-0.3931	-0.0893	C	-4.3850	-1.4322	0.3787	H	1.8543	2.6508	-0.6793
C	4.1945	-1.7682	-0.3937	C	-5.5022	-0.5949	0.4268	H	1.1895	-4.0639	-0.2393
C	2.9317	-2.2677	-0.3986	C	-5.3604	0.7701	0.2734	H	-1.0659	-5.0592	0.0240
C	1.9695	-0.0370	-0.1032	C	-1.5239	2.4478	-0.3218	H	-3.0693	-3.5930	0.2524
C	1.7995	-1.4178	-0.2185	C	-1.6475	1.0641	-0.1304	H	-4.5040	-2.5214	0.4860
C	0.7911	0.8105	-0.2101	C	-2.9522	0.4915	0.0462	H	-6.4947	-1.0305	0.5824
C	-0.2424	2.9940	-0.5437	C	-4.0854	1.3301	0.0765	H	-6.2378	1.4261	0.3030
C	0.8720	2.1960	-0.4905	C	-3.9207	2.7456	-0.1011	H	-4.8150	3.3788	-0.0741
C	0.4804	-2.0178	-0.1448	C	-2.6919	3.2807	-0.3019	H	-2.5617	4.3593	-0.4465
C	0.3089	-3.4126	-0.1354	H	6.9879	1.7462	0.6008				
C	-0.9473	-3.9708	0.0087	H	6.5707	-0.5937	-0.1428				

Table 3.398: Table of thermodynamic data as a function of temperature for Benzo[*pqr*]naphtho[1,2-*b*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K_f</i>
0	0.0	0.0	∞	-53.444	476.350	476.350	∞
100	113.683	356.529	821.994	-46.546	503.278	551.062	-287.840
200	233.044	470.013	617.474	-29.492	489.000	604.549	-157.889
250	301.659	529.338	593.880	-16.135	482.309	634.209	-132.508
298.15	368.380	588.190	588.190	0.000	476.350	664.021	-116.331
300	370.912	590.477	588.197	0.684	476.130	665.183	-115.816
350	437.499	652.704	592.960	20.911	470.635	697.139	-104.040
400	499.297	715.219	604.336	44.353	465.861	729.821	-95.303
450	555.325	777.321	620.113	70.744	461.724	763.070	-88.573
500	605.429	838.475	638.901	99.787	458.131	796.772	-83.236
600	689.427	956.588	682.092	164.697	452.269	865.080	-75.310
700	755.744	1068.040	729.350	237.083	447.962	934.250	-69.713
800	808.788	1172.545	778.289	315.405	445.029	1003.924	-65.548
900	851.885	1270.379	827.590	398.510	443.293	1073.885	-62.325
1000	887.382	1362.030	876.501	485.529	442.589	1143.997	-59.755
1100	916.948	1448.035	924.590	575.790	442.718	1214.149	-57.654
1200	941.794	1528.916	971.614	668.762	443.536	1284.237	-55.900
1300	962.833	1605.153	1017.444	764.022	444.858	1354.248	-54.413
1400	980.768	1677.180	1062.020	861.225	446.549	1424.146	-53.134
1500	996.147	1745.384	1105.324	960.090	448.530	1493.916	-52.022
1600	1009.409	1810.108	1147.368	1060.384	450.666	1563.537	-51.043
1700	1020.907	1871.656	1188.178	1161.913	452.884	1632.996	-50.175
1800	1030.923	1930.299	1227.790	1264.516	455.104	1702.394	-49.401
1900	1039.691	1986.279	1266.249	1368.056	457.299	1771.611	-48.704
2000	1047.401	2039.808	1303.598	1472.419	459.411	1840.743	-48.074
2100	1054.209	2091.079	1339.885	1577.507	461.361	1909.758	-47.502
2200	1060.246	2140.263	1375.156	1683.235	463.147	1978.686	-46.979
2300	1065.620	2187.514	1409.455	1789.534	464.768	2047.537	-46.500
2400	1070.421	2232.969	1442.828	1896.340	466.146	2116.268	-46.058
2500	1074.726	2276.755	1475.314	2003.601	467.298	2185.071	-45.654
2600	1078.598	2318.983	1506.956	2111.271	468.183	2253.704	-45.277
2700	1082.093	2359.756	1537.790	2219.308	468.809	2322.390	-44.928
2800	1085.256	2399.168	1567.854	2327.678	469.147	2391.079	-44.605
2900	1088.127	2437.302	1597.181	2436.350	469.166	2459.704	-44.303
3000	1090.741	2474.236	1625.804	2545.295	468.916	2528.363	-44.022
3100	1093.126	2510.040	1653.753	2654.491	468.311	2596.950	-43.757
3200	1095.309	2544.781	1681.057	2763.914	467.398	2665.643	-43.511
3300	1097.310	2578.516	1707.745	2873.546	466.158	2734.413	-43.281
3400	1099.149	2611.302	1733.840	2983.370	464.561	2803.129	-43.064
3500	1100.843	2643.188	1759.368	3093.371	462.611	2871.878	-42.860
3600	1102.407	2674.222	1784.351	3203.535	460.335	2940.785	-42.669
3700	1103.852	2704.447	1808.812	3313.849	457.697	3009.776	-42.490
3800	1105.192	2733.903	1832.771	3424.302	454.670	3078.780	-42.320
3900	1106.435	2762.627	1856.246	3534.884	451.298	3147.809	-42.159
4000	1107.591	2790.654	1879.258	3645.586	447.564	3217.084	-42.010
4100	1108.667	2818.017	1901.822	3756.399	443.430	3286.375	-41.868
4200	1109.671	2844.745	1923.955	3867.317	438.925	3355.761	-41.734
4300	1110.609	2870.867	1945.674	3978.331	434.036	3425.161	-41.607
4400	1111.486	2896.410	1966.992	4089.437	428.771	3494.779	-41.487
4500	1112.308	2921.397	1987.925	4200.627	423.147	3564.581	-41.376
4600	1113.079	2945.853	2008.484	4311.897	417.107	3634.525	-41.270
4700	1113.803	2969.799	2028.684	4423.241	410.667	3704.478	-41.170
4800	1114.484	2993.256	2048.536	4534.656	403.878	3774.688	-41.076
4900	1115.125	3016.242	2068.051	4646.136	396.659	3844.895	-40.986
5000	1115.729	3038.777	2087.241	4757.679	389.112	3915.457	-40.904

3.399. Benzo[*lm*]naphtho[1,8-*ab*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 97938-05-1
Point Group: C₁

Length: 15.82 Å
Width: 11.59 Å
Breadth: 5.091 Å
L/B Ratio: 1.366

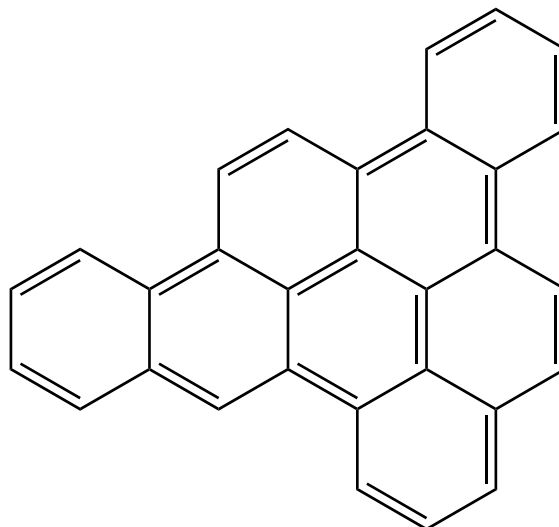
Cartesian coordinates:

C	-2.2535	-3.0406	0.0744	C	4.3278	-0.5341	-0.1027	H	0.9613	-4.1073	-0.2861
C	-1.1716	-3.9237	-0.0739	C	-0.7427	-1.1337	-0.0630	H	2.5617	3.6314	0.8018
C	0.1011	-3.4287	-0.1817	C	-0.5183	0.2834	-0.0675	H	0.2584	2.8180	0.6164
C	0.3427	-2.0319	-0.1491	C	-2.0572	-1.6732	0.0743	H	6.4832	-0.7168	-0.2009
C	0.7822	0.7533	0.1109	C	-1.6880	1.1490	-0.2560	H	6.8895	1.6979	0.2125
C	2.3593	2.5865	0.5390	C	-1.5942	2.4505	-0.7078	H	4.9840	3.2494	0.5606
C	1.0956	2.1297	0.4331	C	-2.7265	3.2864	-0.7994	H	2.5988	-3.4653	-0.5127
C	3.4872	1.7143	0.3235	C	-3.9621	2.8261	-0.4371	H	4.9274	-2.5964	-0.4746
C	5.6406	-0.0317	-0.0542	C	-2.9946	0.6193	-0.0109	H	-0.6200	2.8749	-0.9869
C	5.8653	1.3119	0.1771	C	-4.1198	1.4710	-0.0434	H	-2.5968	4.3150	-1.1521
C	4.7937	2.1871	0.3703	C	-5.4021	0.9588	0.2853	H	-4.8411	3.4798	-0.4647
C	3.2362	0.3419	0.0774	C	-5.5592	-0.3697	0.5799	H	-6.2596	1.6411	0.2934
C	1.8904	-0.1538	0.0123	C	-4.4563	-1.2430	0.5216	H	-6.5434	-0.7701	0.8440
C	1.6793	-1.5226	-0.1748	C	-3.1945	-0.7707	0.2212	H	-4.6023	-2.3201	0.6963
C	2.8014	-2.3951	-0.3545	H	-3.2721	-3.4394	0.1997				
C	4.0736	-1.9249	-0.3290	H	-1.3556	-5.0028	-0.0926				

Table 3.399: Table of thermodynamic data as a function of temperature for Benzo[*lm*]naphtho[1,8-*ab*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.480	512.273	512.273	∞
100	113.372	354.289	820.941	-46.665	539.081	587.090	-306.658
200	233.749	467.903	615.835	-29.586	524.828	640.799	-167.356
250	302.643	527.418	592.165	-16.187	518.180	670.560	-140.103
298.15	369.512	586.457	586.457	0.000	512.273	700.460	-122.715
300	372.047	588.751	586.464	0.686	512.054	701.625	-122.161
350	438.699	651.159	591.241	20.971	506.618	733.663	-109.491
400	500.507	713.835	602.649	44.474	501.905	766.418	-100.082
450	556.508	776.078	618.468	70.925	497.827	799.732	-92.829
500	606.566	837.354	637.302	100.026	494.293	833.493	-87.073
600	690.448	955.665	680.591	165.044	488.539	901.904	-78.516
700	756.647	1067.265	727.942	237.527	484.327	971.158	-72.467
800	809.585	1171.884	776.968	315.933	481.480	1040.904	-67.963
900	852.591	1269.807	826.347	399.114	479.818	1110.926	-64.475
1000	888.011	1361.528	875.329	486.199	479.182	1181.092	-61.693
1100	917.509	1447.589	923.481	576.519	479.369	1251.291	-59.418
1200	942.298	1528.517	970.563	669.544	480.241	1321.421	-57.519
1300	963.287	1604.792	1016.444	764.852	481.611	1391.470	-55.909
1400	981.178	1676.851	1061.067	862.099	483.345	1461.403	-54.524
1500	996.519	1745.082	1104.414	961.003	485.365	1531.204	-53.320
1600	1009.748	1809.829	1146.496	1061.332	487.537	1600.854	-52.261
1700	1021.216	1871.397	1187.341	1162.894	489.786	1670.340	-51.322
1800	1031.206	1930.057	1226.987	1265.526	492.037	1739.763	-50.486
1900	1039.951	1986.051	1265.475	1369.094	494.258	1809.003	-49.732
2000	1047.640	2039.593	1302.852	1473.481	496.396	1878.158	-49.051
2100	1054.430	2090.875	1339.165	1578.592	498.368	1947.194	-48.433
2200	1060.451	2140.069	1374.459	1684.342	500.176	2016.141	-47.868
2300	1065.810	2187.328	1408.781	1790.660	501.816	2085.011	-47.351
2400	1070.598	2232.792	1442.173	1897.485	503.213	2153.761	-46.874
2500	1074.890	2276.584	1474.679	2004.763	504.381	2222.580	-46.437
2600	1078.752	2318.819	1506.339	2112.448	505.283	2291.231	-46.030
2700	1082.237	2359.598	1537.190	2220.501	505.923	2359.933	-45.655
2800	1085.391	2399.014	1567.270	2328.885	506.275	2428.637	-45.306
2900	1088.254	2437.153	1596.612	2437.569	506.308	2497.277	-44.980
3000	1090.860	2474.091	1625.249	2546.527	506.069	2565.951	-44.676
3100	1093.239	2509.899	1653.211	2655.734	505.476	2634.552	-44.391
3200	1095.415	2544.643	1680.528	2765.168	504.574	2703.259	-44.125
3300	1097.410	2578.382	1707.227	2874.811	503.345	2772.043	-43.877
3400	1099.244	2611.170	1733.334	2984.645	501.757	2840.772	-43.642
3500	1100.933	2643.059	1758.872	3094.655	499.817	2909.534	-43.422
3600	1102.492	2674.096	1783.866	3204.827	497.549	2978.454	-43.215
3700	1103.933	2704.323	1808.337	3315.149	494.920	3047.458	-43.022
3800	1105.269	2733.781	1832.304	3425.610	491.900	3116.474	-42.838
3900	1106.508	2762.507	1855.789	3536.200	488.536	3185.515	-42.664
4000	1107.661	2790.536	1878.809	3646.909	484.809	3254.801	-42.502
4100	1108.734	2817.900	1901.381	3757.729	480.682	3324.104	-42.349
4200	1109.735	2844.630	1923.522	3868.653	476.184	3393.502	-42.204
4300	1110.670	2870.754	1945.248	3979.674	471.300	3462.914	-42.065
4400	1111.545	2896.298	1966.574	4090.785	466.042	3532.543	-41.936
4500	1112.364	2921.287	1987.513	4201.981	460.424	3602.356	-41.814
4600	1113.133	2945.744	2008.079	4313.256	454.389	3672.311	-41.700
4700	1113.854	2969.691	2028.285	4424.606	447.954	3742.274	-41.590
4800	1114.533	2993.148	2048.143	4536.026	441.170	3812.496	-41.488
4900	1115.172	3016.136	2067.664	4647.511	433.956	3882.713	-41.389
5000	1115.775	3038.672	2086.860	4759.059	426.413	3953.285	-41.299

3.400. Benzo[*rst*]naphtho[2,1,8-*fgh*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-64-5
Point Group: C_s

Length: 15.91 Å
Width: 11.65 Å
Breadth: 3.887 Å
L/B Ratio: 1.365

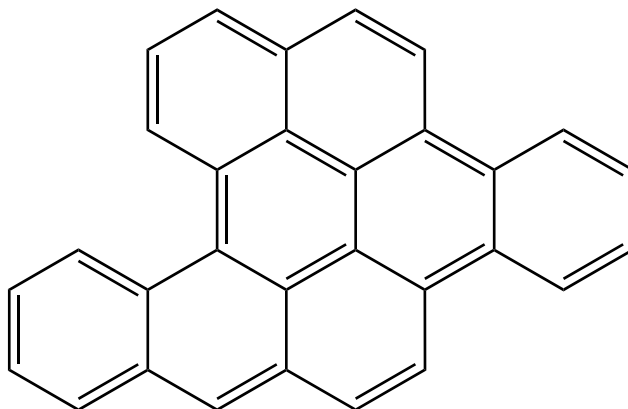
Cartesian coordinates:

C	0.9701	0.2538	0.0000	C	-3.5603	-1.6624	0.0000	H	5.5766	-1.3324	0.0000
C	1.5305	-1.0718	0.0000	C	-2.7073	-0.5183	0.0000	H	3.7237	3.2983	0.0000
C	2.8892	-1.2379	0.0000	C	-0.9757	1.7375	0.0000	H	3.3162	-2.2542	0.0000
C	3.7755	-0.1205	0.0000	C	-2.4092	1.9306	0.0000	H	-3.7089	-3.7975	0.0000
C	3.2515	1.1844	0.0000	C	-3.2656	0.8155	0.0000	H	-4.6484	-1.4962	0.0000
C	1.8221	1.3680	0.0000	C	1.1277	-3.5174	0.0000	H	2.2170	-3.6770	0.0000
C	5.1780	-0.3116	0.0000	C	0.2625	-4.6231	0.0000	H	0.6855	-5.6331	0.0000
C	6.0246	0.7699	0.0000	C	-1.0987	-4.4386	0.0000	H	-1.7802	-5.2967	0.0000
C	5.5030	2.0776	0.0000	C	-4.6625	1.0230	0.0000	H	-5.3255	0.1445	0.0000
C	4.1447	2.2812	0.0000	C	-5.1882	2.2944	0.0000	H	-6.2727	2.4444	0.0000
C	-0.4439	0.4446	0.0000	C	-4.3333	3.4074	0.0000	H	-4.7578	4.4166	0.0000
C	-1.3259	-0.6950	0.0000	C	-2.9694	3.2269	0.0000	H	-2.2909	4.0936	0.0000
C	-0.7744	-2.0166	0.0000	C	1.2597	2.6710	0.0000	H	-0.5275	3.8613	0.0000
C	0.6326	-2.2247	0.0000	C	-0.0940	2.8495	0.0000	H	1.9448	3.5328	0.0000
C	-1.6369	-3.1309	0.0000	H	6.1900	2.9301	0.0000				
C	-3.0485	-2.9228	0.0000	H	7.1098	0.6247	0.0000				

Table 3.400: Table of thermodynamic data as a function of temperature for Benzo[*rst*]naphtho[2,1,8-*fgh*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-54.335	462.547	462.547	∞
100	117.856	371.493	841.100	-46.961	489.060	535.348	-279.631
200	234.955	487.158	635.184	-29.605	475.083	587.203	-153.359
250	302.756	546.816	611.514	-16.174	468.466	615.997	-128.703
298.15	368.935	605.812	605.812	0.000	462.547	644.963	-112.993
300	371.450	608.102	605.819	0.685	462.327	646.093	-112.492
350	437.670	670.383	610.587	20.929	456.849	677.166	-101.059
400	499.233	732.904	621.970	44.374	452.078	708.964	-92.579
450	555.115	794.989	637.752	70.757	447.933	741.328	-86.049
500	605.130	856.116	656.542	99.787	444.328	774.148	-80.873
600	689.052	974.166	699.728	164.663	438.432	840.696	-73.188
700	755.356	1085.559	746.973	237.011	434.085	908.110	-67.763
800	808.413	1190.013	795.896	315.294	431.115	976.035	-63.727
900	851.532	1287.805	845.179	398.363	429.342	1044.252	-60.606
1000	887.056	1379.420	894.072	485.348	428.605	1112.623	-58.116
1100	916.647	1465.395	942.143	575.577	428.702	1181.037	-56.082
1200	941.518	1546.250	989.150	668.520	429.491	1249.391	-54.383
1300	962.580	1622.466	1034.964	763.754	430.786	1317.669	-52.944
1400	980.535	1694.476	1079.524	860.933	432.454	1385.837	-51.705
1500	995.934	1762.664	1122.814	959.776	434.412	1453.878	-50.627
1600	1009.214	1827.375	1164.844	1060.049	436.528	1521.772	-49.680
1700	1020.726	1888.911	1205.641	1161.560	438.726	1589.505	-48.839
1800	1030.757	1947.545	1245.242	1264.145	440.930	1657.177	-48.089
1900	1039.538	2003.515	1283.689	1367.669	443.108	1724.671	-47.414
2000	1047.259	2057.037	1321.028	1472.017	445.206	1792.080	-46.803
2100	1054.078	2108.302	1357.306	1577.091	447.142	1859.372	-46.248
2200	1060.124	2157.480	1392.567	1682.807	448.916	1926.578	-45.742
2300	1065.506	2204.725	1426.858	1789.094	450.524	1993.707	-45.278
2400	1070.315	2250.176	1460.222	1895.889	451.892	2060.718	-44.849
2500	1074.627	2293.957	1492.701	2003.140	453.033	2127.800	-44.457
2600	1078.506	2336.182	1524.336	2110.800	453.909	2194.713	-44.091
2700	1082.006	2376.952	1555.163	2218.829	454.525	2261.679	-43.754
2800	1085.175	2416.360	1585.221	2327.190	454.855	2328.649	-43.441
2900	1088.051	2454.491	1614.542	2435.854	454.867	2395.555	-43.148
3000	1090.669	2491.423	1643.159	2544.792	454.609	2462.495	-42.875
3100	1093.058	2527.225	1671.102	2653.980	453.997	2529.363	-42.619
3200	1095.244	2561.963	1698.402	2763.397	453.078	2596.338	-42.380
3300	1097.249	2595.697	1725.084	2873.023	451.832	2663.390	-42.157
3400	1099.091	2628.481	1751.174	2982.841	450.228	2730.388	-41.946
3500	1100.788	2660.365	1776.698	3092.836	448.273	2797.419	-41.748
3600	1102.355	2691.398	1801.677	3202.995	445.991	2864.608	-41.564
3700	1103.803	2721.621	1826.134	3313.303	443.348	2931.882	-41.390
3800	1105.145	2751.076	1850.089	3423.752	440.316	2999.169	-41.226
3900	1106.390	2779.799	1873.561	3534.329	436.940	3066.481	-41.070
4000	1107.548	2807.825	1896.568	3645.027	433.201	3134.038	-40.925
4100	1108.626	2835.187	1919.129	3755.836	429.063	3201.612	-40.788
4200	1109.632	2861.914	1941.259	3866.750	424.554	3269.282	-40.659
4300	1110.572	2888.035	1962.975	3977.760	419.661	3336.965	-40.535
4400	1111.451	2913.577	1984.290	4088.862	414.393	3404.866	-40.420
4500	1112.274	2938.564	2005.220	4200.049	408.765	3472.951	-40.312
4600	1113.046	2963.019	2025.776	4311.315	402.722	3541.178	-40.211
4700	1113.771	2986.964	2045.973	4422.656	396.279	3609.414	-40.113
4800	1114.453	3010.420	2065.823	4534.068	389.487	3677.909	-40.023
4900	1115.096	3033.406	2085.335	4645.546	382.264	3746.399	-39.936
5000	1115.701	3055.940	2104.523	4757.086	374.714	3815.244	-39.857

3.401. Benzo[*a*]naphtho[1,2,3,4-*ghi*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-76-9
Point Group: C₁

Length: 15.88 Å
Width: 11.62 Å
Breadth: 4.934 Å
L/B Ratio: 1.367

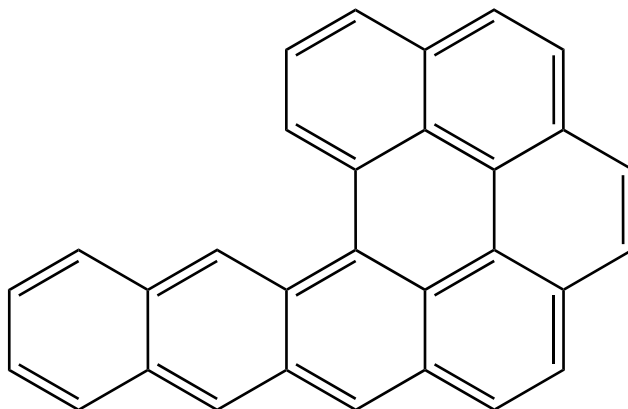
Cartesian coordinates:

C	5.4066	0.0321	-0.7168	C	1.8305	3.8052	0.5568	H	4.9876	-3.2489	0.1022
C	5.7388	-1.3200	-0.4473	C	2.2258	2.4614	0.5180	H	3.8959	1.5265	-0.7902
C	4.7585	-2.1937	-0.0872	C	-0.6753	-0.5924	0.1148	H	2.6669	-3.7541	0.4499
C	4.1275	0.4774	-0.5605	C	-1.0527	0.7839	-0.0208	H	0.3248	-4.3468	0.5667
C	3.0739	-0.3860	-0.1250	C	-0.0419	1.7937	0.0599	H	-2.0703	-3.7037	0.4115
C	3.4029	-1.7574	0.0404	C	1.3329	1.4457	0.2042	H	-3.8048	2.7745	-0.4249
C	2.3985	-2.7014	0.2960	C	1.7311	0.0416	0.0839	H	-2.0757	4.5511	-0.2066
C	1.0677	-2.3130	0.3031	C	0.7235	-0.9373	0.1786	H	0.2196	5.2085	0.2865
C	0.0305	-3.3005	0.4237	C	-3.4094	0.1192	-0.1790	H	2.5738	4.5738	0.7942
C	-1.2726	-2.9486	0.3418	C	-3.0442	-1.2281	-0.0016	H	3.2777	2.2292	0.7342
C	-1.6563	-1.5788	0.1544	C	-4.0585	-2.2166	0.0086	H	-3.7668	-3.2678	0.1539
C	-2.3944	1.1395	-0.1655	C	-5.3777	-1.8768	-0.1595	H	-6.1546	-2.6482	-0.1513
C	-2.7454	2.5205	-0.2676	C	-5.7409	-0.5301	-0.3450	H	-6.7955	-0.2697	-0.4813
C	-1.8023	3.4912	-0.1512	C	-4.7761	0.4461	-0.3528	H	-5.0480	1.5033	-0.4934
C	-0.4302	3.1498	0.0580	H	6.1933	0.7119	-1.0608				
C	0.5282	4.1572	0.2928	H	6.7787	-1.6464	-0.5484				

Table 3.401: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[1,2,3,4-*ghi*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.719	497.734	497.734	∞
100	114.936	357.698	825.216	-46.752	524.456	572.124	-298.841
200	234.073	472.028	619.913	-29.577	510.299	625.445	-163.346
250	302.510	531.562	596.256	-16.173	503.655	654.999	-136.852
298.15	369.111	590.554	590.554	0.000	497.734	684.700	-119.954
300	371.639	592.845	590.561	0.685	497.515	685.858	-119.416
350	438.135	655.177	595.331	20.946	492.054	717.693	-107.108
400	499.861	717.772	606.725	44.419	487.311	750.249	-97.970
450	555.827	779.937	622.524	70.836	483.200	783.368	-90.929
500	605.877	841.140	641.336	99.902	479.631	816.938	-85.343
600	689.785	959.327	684.572	164.853	473.809	884.977	-77.042
700	756.031	1070.829	731.870	237.271	469.533	953.870	-71.177
800	809.020	1175.369	780.845	315.619	466.627	1023.263	-66.811
900	852.073	1273.228	830.178	398.745	464.911	1092.941	-63.431
1000	887.536	1364.896	879.115	485.781	464.225	1162.767	-60.735
1100	917.075	1450.915	927.228	576.055	464.368	1232.631	-58.532
1200	941.900	1531.806	974.273	669.039	465.197	1302.431	-56.692
1300	962.923	1608.051	1020.121	764.309	466.529	1372.152	-55.133
1400	980.843	1680.084	1064.712	861.520	468.229	1441.760	-53.792
1500	996.212	1748.293	1108.031	960.393	470.217	1511.240	-52.625
1600	1009.466	1813.020	1150.087	1060.692	472.359	1580.570	-51.599
1700	1020.955	1874.572	1190.909	1162.227	474.581	1649.737	-50.689
1800	1030.966	1933.218	1230.532	1264.834	476.806	1718.843	-49.879
1900	1039.729	1989.199	1269.000	1368.379	479.005	1787.769	-49.148
2000	1047.434	2042.730	1306.358	1472.745	481.121	1856.609	-48.489
2100	1054.239	2094.003	1342.652	1577.835	483.074	1925.331	-47.889
2200	1060.273	2143.188	1377.930	1683.567	484.863	1993.966	-47.342
2300	1065.644	2190.440	1412.236	1789.868	486.486	2062.525	-46.840
2400	1070.443	2235.896	1445.614	1896.677	487.867	2130.964	-46.378
2500	1074.746	2279.683	1478.107	2003.940	489.020	2199.473	-45.955
2600	1078.617	2321.912	1509.754	2111.612	489.908	2267.814	-45.560
2700	1082.110	2362.686	1540.593	2219.651	490.535	2336.207	-45.196
2800	1085.272	2402.098	1570.661	2328.023	490.875	2404.603	-44.857
2900	1088.142	2440.232	1599.992	2436.696	490.896	2472.935	-44.541
3000	1090.755	2477.167	1628.619	2545.642	490.647	2541.301	-44.247
3100	1093.139	2512.972	1656.572	2654.839	490.043	2609.594	-43.970
3200	1095.320	2547.712	1683.880	2764.263	489.132	2677.994	-43.713
3300	1097.321	2581.448	1710.570	2873.897	487.893	2746.471	-43.472
3400	1099.159	2614.234	1736.669	2983.722	486.296	2814.894	-43.245
3500	1100.853	2646.121	1762.200	3093.724	484.348	2883.350	-43.031
3600	1102.416	2677.155	1787.186	3203.888	482.073	2951.964	-42.831
3700	1103.861	2707.380	1811.650	3314.203	479.435	3020.661	-42.643
3800	1105.200	2736.836	1835.611	3424.657	476.409	3089.372	-42.466
3900	1106.443	2765.561	1859.089	3535.240	473.038	3158.108	-42.297
4000	1107.598	2793.588	1882.102	3645.943	469.305	3227.089	-42.141
4100	1108.674	2820.951	1904.669	3756.757	465.171	3296.086	-41.992
4200	1109.678	2847.679	1926.804	3867.675	460.667	3365.180	-41.851
4300	1110.615	2873.802	1948.525	3978.690	455.778	3434.286	-41.717
4400	1111.492	2899.344	1969.845	4089.796	450.514	3503.611	-41.592
4500	1112.314	2924.332	1990.780	4200.987	444.891	3573.119	-41.475
4600	1113.084	2948.788	2011.341	4312.257	438.851	3642.769	-41.364
4700	1113.808	2972.734	2031.542	4423.602	432.412	3712.429	-41.258
4800	1114.489	2996.191	2051.396	4535.017	425.623	3782.346	-41.159
4900	1115.129	3019.177	2070.912	4646.498	418.405	3852.259	-41.065
5000	1115.733	3041.712	2090.104	4758.042	410.858	3922.527	-40.978

3.402. Benzo[uv]naphtho[2,1,8,7-defg]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-86-1
Point Group: C₁

Length: 15.94 Å
Width: 11.62 Å
Breadth: 5.056 Å
L/B Ratio: 1.372

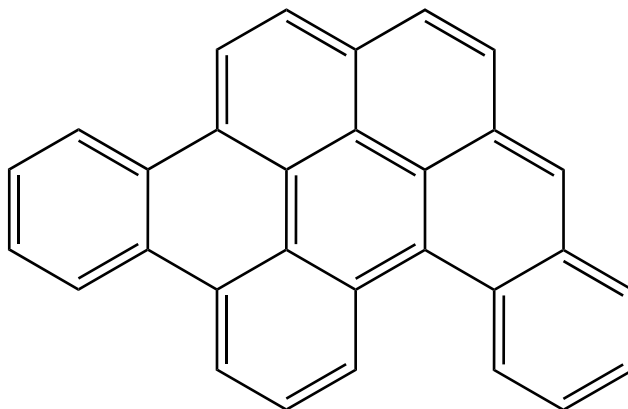
Cartesian coordinates:

C	6.0532	1.2715	-0.5988	C	-4.9666	-0.7117	-0.4899	H	6.0603	-2.0488	0.2391
C	6.5483	-0.0312	-0.2925	C	-2.2106	-1.0132	-0.0218	H	4.3298	2.5225	-0.8243
C	5.6922	-1.0436	0.0050	C	0.0599	-0.0465	0.1801	H	3.7365	-2.8576	0.4545
C	4.7180	1.5249	-0.5893	C	-0.7854	-1.1571	0.1487	H	2.0619	1.7466	-0.4685
C	3.7822	0.4857	-0.2677	C	-0.5457	1.2790	0.2926	H	1.4949	-3.6929	0.5589
C	4.2761	-0.8159	0.0177	C	-1.7657	3.8343	0.3844	H	-0.7320	-4.6169	0.3845
C	3.3695	-1.8396	0.2720	C	-0.4379	3.6734	0.7314	H	-3.1698	-4.3124	0.0286
C	2.4112	0.7316	-0.2286	C	0.1601	2.4147	0.6914	H	-5.0649	-2.8569	-0.4240
C	1.4842	-0.2704	0.0943	C	-2.5357	2.7086	0.0582	H	-6.0382	-0.5883	-0.6840
C	1.9885	-1.5924	0.2763	C	-1.9386	1.4288	0.0528	H	-2.2262	4.8286	0.3850
C	1.0894	-2.6855	0.4010	C	-2.7732	0.2806	-0.1364	H	0.1559	4.5404	1.0403
C	-0.2613	-2.4881	0.2689	C	-4.1522	0.4313	-0.3714	H	1.2165	2.3352	0.9833
C	-1.1643	-3.6181	0.2521	C	-4.7099	1.7517	-0.4572	H	-5.7773	1.8506	-0.6850
C	-2.4885	-3.4545	0.0610	C	-3.9353	2.8416	-0.2437	H	-4.3582	3.8519	-0.2894
C	-3.0482	-2.1356	-0.1050	H	6.7721	2.0610	-0.8412				
C	-4.4254	-1.9698	-0.3481	H	7.6306	-0.1962	-0.3042				

Table 3.402: Table of thermodynamic data as a function of temperature for Benzo[uv]naphtho[2,1,8,7-defg]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.263	496.963	496.963	∞
100	112.277	353.097	818.168	-46.507	523.930	572.058	-298.806
200	232.959	465.995	613.643	-29.530	509.575	625.927	-163.472
250	302.084	525.360	590.013	-16.163	502.893	655.789	-137.017
298.15	369.083	584.313	584.313	0.000	496.963	685.789	-120.145
300	371.622	586.604	584.320	0.685	496.744	686.959	-119.608
350	438.322	648.951	589.092	20.951	491.288	719.106	-107.318
400	500.134	711.578	600.489	44.435	486.556	751.972	-98.195
450	556.128	773.777	616.295	70.867	482.460	785.400	-91.165
500	606.183	835.012	635.114	99.949	478.906	819.278	-85.588
600	690.093	953.255	678.371	164.930	473.115	887.926	-77.299
700	756.354	1064.805	725.691	237.380	468.870	957.424	-71.442
800	809.367	1169.389	774.689	315.761	465.997	1027.417	-67.082
900	852.444	1267.291	824.043	398.923	464.318	1097.690	-63.707
1000	887.925	1359.000	873.003	485.997	463.670	1168.108	-61.014
1100	917.472	1445.055	921.137	576.311	463.851	1238.560	-58.813
1200	942.297	1525.981	968.202	669.334	464.721	1308.944	-56.976
1300	963.314	1602.258	1014.070	764.643	466.092	1379.247	-55.418
1400	981.224	1674.320	1058.681	861.894	467.830	1449.433	-54.078
1500	996.578	1742.554	1102.019	960.803	469.856	1519.487	-52.912
1600	1009.816	1807.304	1144.093	1061.139	472.034	1589.390	-51.887
1700	1021.289	1868.877	1184.931	1162.707	474.290	1659.128	-50.978
1800	1031.282	1927.541	1224.570	1265.347	476.548	1728.802	-50.168
1900	1040.028	1983.539	1263.054	1368.922	478.777	1798.294	-49.438
2000	1047.717	2037.085	1300.426	1473.318	480.922	1867.700	-48.778
2100	1054.506	2088.371	1336.735	1578.436	482.902	1936.986	-48.179
2200	1060.525	2137.568	1372.026	1684.193	484.718	2006.184	-47.632
2300	1065.882	2184.831	1406.345	1790.519	486.365	2075.304	-47.131
2400	1070.667	2230.298	1439.735	1897.350	487.769	2144.303	-46.669
2500	1074.957	2274.093	1472.239	2004.635	488.944	2213.372	-46.245
2600	1078.816	2316.330	1503.896	2112.327	489.852	2282.271	-45.850
2700	1082.298	2357.111	1534.746	2220.386	490.499	2351.222	-45.486
2800	1085.450	2396.530	1564.824	2328.776	490.857	2420.175	-45.148
2900	1088.311	2434.670	1594.165	2437.467	490.895	2489.064	-44.832
3000	1090.915	2471.610	1622.801	2546.430	490.663	2557.985	-44.538
3100	1093.291	2507.421	1650.762	2655.642	490.075	2626.834	-44.261
3200	1095.465	2542.166	1678.078	2765.081	489.178	2695.789	-44.003
3300	1097.458	2575.906	1704.776	2874.729	487.954	2764.821	-43.763
3400	1099.290	2608.696	1730.882	2984.567	486.370	2833.797	-43.535
3500	1100.977	2640.587	1756.420	3094.582	484.435	2902.807	-43.321
3600	1102.534	2671.624	1781.414	3204.758	482.171	2971.974	-43.121
3700	1103.974	2701.852	1805.884	3315.085	479.546	3041.224	-42.934
3800	1105.308	2731.311	1829.851	3425.550	476.530	3110.488	-42.756
3900	1106.546	2760.038	1853.335	3536.143	473.170	3179.776	-42.587
4000	1107.697	2788.068	1876.354	3646.856	469.447	3249.309	-42.431
4100	1108.768	2815.434	1898.926	3757.680	465.323	3318.858	-42.282
4200	1109.768	2842.164	1921.068	3868.607	460.828	3388.503	-42.141
4300	1110.702	2868.289	1942.793	3979.631	455.948	3458.161	-42.007
4400	1111.575	2893.834	1964.119	4090.746	450.692	3528.037	-41.882
4500	1112.393	2918.823	1985.058	4201.944	445.077	3598.096	-41.765
4600	1113.161	2943.281	2005.624	4313.222	439.045	3668.297	-41.654
4700	1113.882	2967.228	2025.829	4424.575	432.614	3738.507	-41.548
4800	1114.559	2990.687	2045.687	4535.997	425.832	3808.975	-41.449
4900	1115.198	3013.675	2065.208	4647.486	418.620	3879.438	-41.354
5000	1115.799	3036.211	2084.404	4759.036	411.080	3950.257	-41.267

3.403. Tribenzo[*a,ghi,k*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-75-8
Point Group: C₁

Length: 15.89 Å
Width: 11.61 Å
Breadth: 5.098 Å
L/B Ratio: 1.369

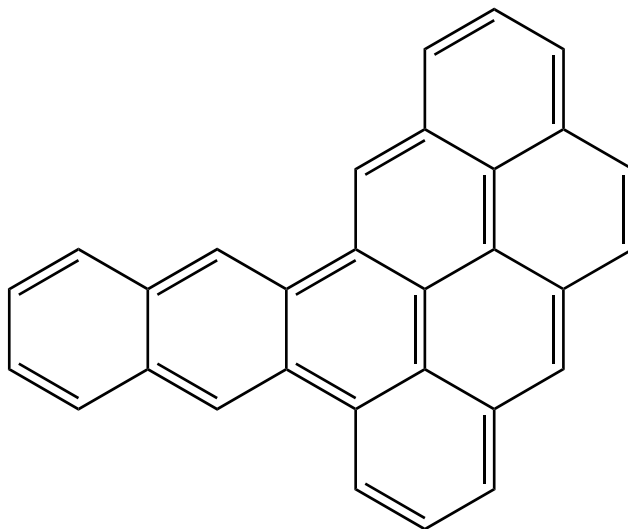
Cartesian coordinates:

C	1.6965	2.9825	-0.4864	C	1.0449	-0.6653	-0.0186	H	0.2566	4.4925	-1.0144
C	-0.6719	2.5876	-0.6316	C	-0.0518	-1.5557	-0.0998	H	3.5773	-2.9431	0.2588
C	0.4152	3.4451	-0.7367	C	-2.9930	0.7756	0.1291	H	1.6615	-4.5158	0.0407
C	1.9103	1.6309	-0.1997	C	-4.0517	-0.1598	0.0201	H	-0.7155	-4.9274	-0.2689
C	2.3490	-1.1708	0.1107	C	-5.4053	0.2641	0.1673	H	-3.0441	-4.0735	-0.3905
C	2.5508	-2.5617	0.1455	C	-5.6978	1.5566	0.4920	H	-4.6101	-2.2332	-0.2980
C	1.4898	-3.4334	0.0299	C	-4.6453	2.4782	0.7029	H	-6.2044	-0.4726	0.0252
C	0.1797	-2.9429	-0.0991	C	-3.3445	2.0994	0.5277	H	-6.7345	1.8881	0.6086
C	-0.9296	-3.8534	-0.2269	C	3.4722	-0.2529	0.1835	H	-4.8872	3.4994	1.0157
C	-2.1941	-3.3885	-0.2910	C	3.2566	1.1252	0.0209	H	-2.5466	2.8313	0.7132
C	-2.4732	-1.9739	-0.2113	C	4.3560	2.0015	0.0781	H	4.1802	3.0796	-0.0586
C	-3.7780	-1.5258	-0.1914	C	5.6319	1.5232	0.2989	H	6.4790	2.2153	0.3447
C	-1.3969	-1.0390	-0.1452	C	5.8452	0.1507	0.4642	H	6.8581	-0.2261	0.6393
C	-1.6474	0.3404	-0.0937	C	4.7793	-0.7242	0.4043	H	4.9360	-1.8070	0.5256
C	-0.5129	1.2457	-0.2685	H	2.5578	3.6663	-0.5286				
C	0.8085	0.7497	-0.1400	H	-1.6738	2.9870	-0.8401				

Table 3.403: Table of thermodynamic data as a function of temperature for Tribenzo[*a,ghi,k*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.600	485.531	485.531	∞
100	114.399	355.307	822.389	-46.708	512.297	560.203	-292.614
200	233.898	469.403	617.228	-29.565	498.108	613.778	-160.299
250	302.390	528.905	593.579	-16.169	491.456	643.465	-134.442
298.15	369.034	587.878	587.878	0.000	485.531	673.294	-117.956
300	371.564	590.169	587.885	0.685	485.312	674.457	-117.431
350	438.103	652.493	592.655	20.943	479.848	706.426	-105.426
400	499.867	715.086	604.048	44.415	475.104	739.117	-96.517
450	555.864	777.254	619.846	70.833	470.994	772.370	-89.653
500	605.937	838.462	638.657	99.903	467.427	806.074	-84.208
600	689.874	956.663	681.895	164.861	461.613	874.379	-76.120
700	756.133	1068.179	729.196	237.288	457.347	943.538	-70.406
800	809.127	1172.733	778.175	315.646	454.451	1013.196	-66.154
900	852.181	1270.605	827.512	398.784	452.746	1083.136	-62.862
1000	887.643	1362.285	876.455	485.830	452.071	1153.224	-60.237
1100	917.178	1448.313	924.572	576.115	452.224	1223.349	-58.091
1200	941.998	1529.213	971.622	669.109	453.064	1293.408	-56.299
1300	963.016	1605.466	1017.475	764.388	454.405	1363.389	-54.781
1400	980.931	1677.506	1062.071	861.609	456.114	1433.255	-53.474
1500	996.294	1745.720	1105.394	960.490	458.110	1502.992	-52.338
1600	1009.543	1810.453	1147.454	1060.797	460.260	1572.579	-51.338
1700	1021.027	1872.009	1188.280	1162.339	462.490	1642.003	-50.452
1800	1031.033	1930.659	1227.907	1264.954	464.722	1711.365	-49.662
1900	1039.792	1986.644	1266.378	1368.504	466.927	1780.546	-48.950
2000	1047.493	2040.178	1303.740	1472.877	469.050	1849.642	-48.307
2100	1054.294	2091.453	1340.037	1577.973	471.008	1918.619	-47.722
2200	1060.325	2140.641	1375.318	1683.710	472.803	1987.509	-47.188
2300	1065.693	2187.895	1409.627	1790.016	474.431	2056.323	-46.700
2400	1070.488	2233.354	1443.008	1896.829	475.816	2125.015	-46.249
2500	1074.788	2277.142	1475.503	2004.097	476.974	2193.779	-45.836
2600	1078.657	2319.372	1507.152	2111.773	477.865	2262.374	-45.451
2700	1082.147	2360.148	1537.994	2219.816	478.497	2331.021	-45.095
2800	1085.307	2399.561	1568.064	2328.191	478.840	2399.670	-44.765
2900	1088.175	2437.697	1597.398	2436.868	478.864	2468.256	-44.457
3000	1090.786	2474.632	1626.026	2545.818	478.618	2536.875	-44.170
3100	1093.169	2510.438	1653.981	2655.017	478.018	2605.423	-43.900
3200	1095.349	2545.180	1681.291	2764.445	477.109	2674.076	-43.649
3300	1097.348	2578.917	1707.983	2874.081	475.874	2742.806	-43.414
3400	1099.185	2611.704	1734.083	2983.909	474.280	2811.482	-43.192
3500	1100.877	2643.591	1759.616	3093.913	472.334	2880.191	-42.984
3600	1102.439	2674.626	1784.604	3204.080	470.061	2949.057	-42.789
3700	1103.883	2704.851	1809.068	3314.397	467.426	3018.008	-42.606
3800	1105.221	2734.308	1833.031	3424.853	464.402	3086.972	-42.433
3900	1106.463	2763.033	1856.510	3535.438	461.032	3155.960	-42.268
4000	1107.617	2791.061	1879.525	3646.142	457.301	3225.194	-42.116
4100	1108.692	2818.424	1902.093	3756.959	453.169	3294.444	-41.971
4200	1109.695	2845.153	1924.230	3867.879	448.667	3363.790	-41.834
4300	1110.632	2871.276	1945.951	3978.895	443.780	3433.149	-41.704
4400	1111.508	2896.819	1967.273	4090.003	438.518	3502.726	-41.582
4500	1112.329	2921.807	1988.208	4201.195	432.896	3572.487	-41.467
4600	1113.099	2946.263	2008.770	4312.467	426.858	3642.390	-41.360
4700	1113.822	2970.210	2028.973	4423.813	420.420	3712.302	-41.257
4800	1114.502	2993.667	2048.827	4535.230	413.633	3782.471	-41.161
4900	1115.142	3016.653	2068.345	4646.712	406.415	3852.637	-41.069
5000	1115.746	3039.189	2087.537	4758.257	398.870	3923.157	-40.984

3.404. Anthra[2,1,9,8-*defgh*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-77-0
Point Group: C_s

Length: 15.92 Å
Width: 11.64 Å
Breadth: 3.887 Å
L/B Ratio: 1.368

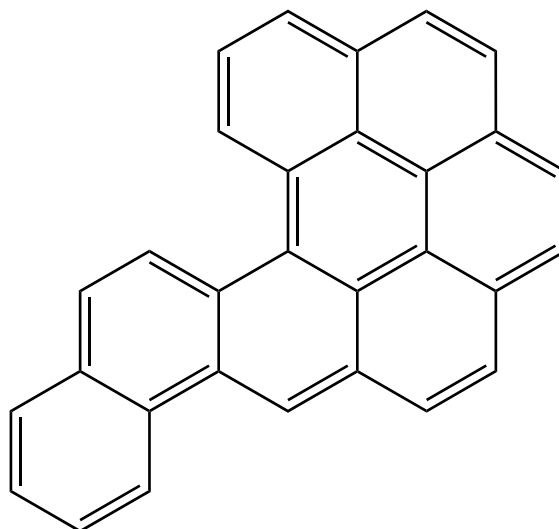
Cartesian coordinates:

C	1.5168	3.2648	0.0000	C	-0.9356	0.4523	0.0000	H	-1.3878	5.0518	0.0000
C	0.6511	4.3727	0.0000	C	-0.0771	-0.7004	0.0000	H	-3.3174	3.5676	0.0000
C	-0.7086	4.1918	0.0000	C	1.0216	1.9741	0.0000	H	-5.2728	2.0873	0.0000
C	-1.2537	2.8834	0.0000	C	-0.3874	1.7686	0.0000	H	-6.2315	-0.1984	0.0000
C	-2.6610	2.6886	0.0000	C	1.9155	0.8171	0.0000	H	-5.9090	-2.6411	0.0000
C	-3.1932	1.4213	0.0000	C	1.3727	-0.5040	0.0000	H	-4.4057	-4.6119	0.0000
C	-4.6249	1.2030	0.0000	C	2.2263	-1.5889	0.0000	H	-1.9407	-4.3206	0.0000
C	-5.1469	-0.0398	0.0000	C	3.2848	0.9903	0.0000	H	0.0327	-2.8416	0.0000
C	-4.2962	-1.2098	0.0000	C	4.1656	-0.1157	0.0000	H	1.8093	-2.6091	0.0000
C	-4.8230	-2.4943	0.0000	C	3.6301	-1.4202	0.0000	H	3.7037	2.0098	0.0000
C	-3.9722	-3.6061	0.0000	C	4.5133	-2.5359	0.0000	H	4.0893	-3.5462	0.0000
C	-2.6015	-3.4465	0.0000	C	5.8668	-2.3416	0.0000	H	6.5517	-3.1958	0.0000
C	-2.8884	-1.0307	0.0000	C	6.4046	-1.0312	0.0000	H	7.4922	-0.9045	0.0000
C	-2.0375	-2.1550	0.0000	C	5.5779	0.0578	0.0000	H	5.9858	1.0748	0.0000
C	-0.6248	-1.9571	0.0000	H	2.6059	3.4263	0.0000				
C	-2.3250	0.2821	0.0000	H	1.0768	5.3816	0.0000				

Table 3.404: Table of thermodynamic data as a function of temperature for Anthra[2,1,9,8-defgh]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-54.034	471.480	471.480	∞
100	115.790	367.439	835.993	-46.855	498.099	544.792	-284.565
200	234.564	482.200	630.302	-29.621	484.002	597.113	-155.947
250	302.962	541.840	606.613	-16.193	477.381	626.156	-130.825
298.15	369.475	600.904	600.904	0.000	471.480	655.360	-114.814
300	371.999	603.197	600.911	0.686	471.262	656.499	-114.304
350	438.368	665.576	605.686	20.961	465.816	687.815	-102.649
400	499.969	728.193	617.087	44.443	461.081	719.851	-94.001
450	555.833	790.365	632.893	70.862	456.972	752.448	-87.340
500	605.813	851.565	651.710	99.928	453.402	785.497	-82.059
600	689.668	969.734	694.953	164.868	447.570	852.494	-74.215
700	755.935	1081.219	742.254	237.275	443.283	920.347	-68.676
800	808.977	1185.749	791.229	315.616	440.370	988.702	-64.554
900	852.090	1283.606	840.561	398.741	438.653	1057.342	-61.365
1000	887.606	1375.280	889.498	485.781	437.971	1126.130	-58.822
1100	917.186	1461.307	937.611	576.065	438.123	1194.955	-56.743
1200	942.041	1542.208	984.657	669.061	438.965	1263.715	-55.007
1300	963.084	1618.466	1030.507	764.346	440.312	1332.396	-53.535
1400	981.016	1690.512	1075.101	861.575	442.029	1400.962	-52.269
1500	996.391	1758.732	1118.423	960.464	444.034	1469.398	-51.168
1600	1009.646	1823.472	1160.483	1060.782	446.194	1537.683	-50.199
1700	1021.135	1885.034	1201.308	1162.335	448.435	1605.805	-49.339
1800	1031.142	1943.690	1240.935	1264.960	450.678	1673.864	-48.573
1900	1039.899	1999.681	1279.406	1368.521	452.894	1741.742	-47.883
2000	1047.599	2053.221	1316.768	1472.904	455.027	1809.534	-47.259
2100	1054.397	2104.501	1353.067	1578.011	456.995	1877.207	-46.692
2200	1060.425	2153.693	1388.349	1683.758	458.800	1944.792	-46.174
2300	1065.789	2200.952	1422.659	1790.074	460.438	2012.299	-45.700
2400	1070.581	2246.414	1456.041	1896.897	461.833	2079.686	-45.262
2500	1074.878	2290.206	1488.537	2004.174	463.000	2147.144	-44.861
2600	1078.742	2332.440	1520.187	2111.858	463.900	2214.432	-44.488
2700	1082.229	2373.219	1551.030	2219.910	464.540	2281.772	-44.143
2800	1085.385	2412.635	1581.102	2328.293	464.891	2349.114	-43.822
2900	1088.250	2450.774	1610.437	2436.977	464.923	2416.392	-43.523
3000	1090.858	2487.712	1639.067	2545.934	464.684	2483.704	-43.244
3100	1093.237	2523.520	1667.023	2655.141	464.091	2550.943	-42.982
3200	1095.414	2558.264	1694.334	2764.575	463.189	2618.288	-42.738
3300	1097.410	2592.002	1721.027	2874.218	461.960	2685.710	-42.510
3400	1099.244	2624.791	1747.129	2984.052	460.372	2753.077	-42.295
3500	1100.934	2656.680	1772.662	3094.062	458.432	2820.477	-42.092
3600	1102.493	2687.716	1797.651	3204.234	456.164	2888.035	-41.903
3700	1103.935	2717.944	1822.117	3314.556	453.534	2955.676	-41.726
3800	1105.271	2747.401	1846.081	3425.018	450.516	3023.330	-41.558
3900	1106.511	2776.128	1869.562	3535.607	447.151	3091.010	-41.399
4000	1107.663	2804.157	1892.578	3646.317	443.425	3158.934	-41.251
4100	1108.737	2831.521	1915.146	3757.137	439.297	3226.874	-41.110
4200	1109.738	2858.251	1937.284	3868.062	434.800	3294.911	-40.977
4300	1110.673	2884.375	1959.007	3979.083	429.917	3362.960	-40.851
4400	1111.547	2909.919	1980.329	4090.194	424.658	3431.227	-40.733
4500	1112.367	2934.908	2001.266	4201.390	419.040	3499.678	-40.622
4600	1113.135	2959.365	2021.829	4312.666	413.006	3568.270	-40.518
4700	1113.857	2983.312	2042.032	4424.016	406.572	3636.872	-40.418
4800	1114.536	3006.770	2061.887	4535.436	399.788	3705.731	-40.326
4900	1115.175	3029.757	2081.406	4646.922	392.574	3774.586	-40.237
5000	1115.777	3052.293	2100.599	4758.470	385.032	3843.797	-40.155

3.405. Benzo[ghi]naphtho[2,1-a]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-59-8
Point Group: C₁

Length: 15.88 Å
Width: 11.62 Å
Breadth: 4.916 Å
L/B Ratio: 1.366

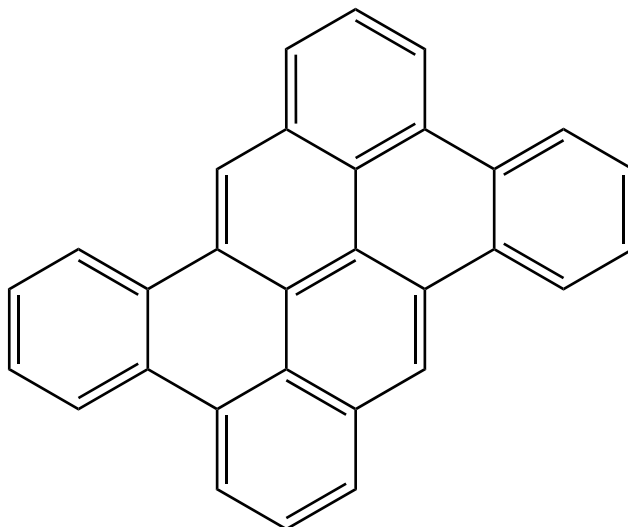
Cartesian coordinates:

C	3.3057	-2.0541	0.5965	C	-1.6015	-3.7471	-0.6015	H	2.5514	2.6304	-0.3806
C	1.9742	-1.8458	0.4902	C	-0.6383	-2.7359	-0.5471	H	0.7172	4.2161	-0.3644
C	1.4186	-0.5759	0.0958	C	-3.3141	-2.1526	-0.0448	H	-1.7092	4.7095	-0.1511
C	2.3232	0.5054	-0.0601	C	-2.3466	-1.1263	-0.0262	H	-3.9912	3.9374	0.2134
C	1.8379	1.8020	-0.2424	C	-2.7881	0.2306	0.0995	H	-5.6364	2.0936	0.4580
C	0.4713	2.0555	-0.2050	C	-4.1503	0.5253	0.2633	H	-3.6739	-4.2727	-0.3287
C	-0.0159	3.4093	-0.2497	C	-5.0976	-0.5483	0.3408	H	-1.2951	-4.7643	-0.8681
C	-1.3364	3.6791	-0.1352	C	-4.6953	-1.8332	0.1848	H	0.4009	-3.0009	-0.7852
C	-2.2864	2.6122	0.0135	C	3.7561	0.2736	-0.0095	H	-6.1515	-0.3017	0.5130
C	-3.6619	2.8923	0.1858	C	4.2418	-1.0054	0.3053	H	-5.4164	-2.6579	0.2220
C	-4.5717	1.8740	0.3190	C	5.6306	-1.2422	0.3484	H	5.9953	-2.2457	0.5951
C	-1.8420	1.2826	-0.0085	C	6.5160	-0.2208	0.0828	H	7.5953	-0.4020	0.1128
C	0.0262	-0.3591	-0.0692	C	6.0372	1.0612	-0.2273	H	6.7484	1.8674	-0.4352
C	-0.4401	0.9745	-0.1089	C	4.6822	1.3051	-0.2704	H	4.3012	2.3096	-0.5091
C	-0.9670	-1.4293	-0.1966	H	3.6995	-3.0265	0.9147				
C	-2.9231	-3.4747	-0.3187	H	1.2839	-2.6643	0.7373				

Table 3.405: Table of thermodynamic data as a function of temperature for Benzo[ghi]naphtho[2,1-a]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.503	477.077	477.077	∞
100	113.367	355.957	822.313	-46.636	503.915	551.757	-288.202
200	233.574	469.456	617.326	-29.574	489.645	605.305	-158.086
250	302.523	528.938	593.665	-16.182	482.989	634.989	-132.671
298.15	369.418	587.959	587.959	0.000	477.077	664.816	-116.471
300	371.954	590.252	587.966	0.686	476.858	665.979	-115.955
350	438.604	652.646	592.741	20.967	471.417	697.942	-104.160
400	500.395	715.308	604.147	44.465	466.699	730.623	-95.408
450	556.380	777.538	619.962	70.909	462.616	763.864	-88.665
500	606.427	838.799	638.793	100.003	459.074	797.552	-83.318
600	690.309	957.084	682.071	165.008	453.306	865.820	-75.375
700	756.532	1068.665	729.412	237.477	449.082	934.933	-69.764
800	809.504	1173.270	778.428	315.874	446.224	1004.539	-65.588
900	852.542	1271.186	827.799	399.048	444.556	1074.424	-62.357
1000	887.990	1362.903	876.773	486.130	443.916	1144.452	-59.779
1100	917.511	1448.964	924.919	576.449	444.103	1214.513	-57.671
1200	942.317	1529.892	971.996	669.475	444.976	1284.506	-55.912
1300	963.318	1606.169	1017.873	764.785	446.348	1354.417	-54.420
1400	981.217	1678.231	1062.492	862.036	448.086	1424.212	-53.137
1500	996.564	1746.465	1105.836	960.944	450.111	1493.875	-52.020
1600	1009.797	1811.214	1147.916	1061.278	452.287	1563.387	-51.038
1700	1021.266	1872.785	1188.759	1162.845	454.541	1632.734	-50.167
1800	1031.257	1931.449	1228.403	1265.482	456.797	1702.018	-49.390
1900	1040.001	1987.445	1266.890	1369.055	459.023	1771.119	-48.690
2000	1047.690	2040.990	1304.266	1473.447	461.166	1840.134	-48.058
2100	1054.478	2092.274	1340.578	1578.562	463.143	1909.030	-47.484
2200	1060.497	2141.470	1375.872	1684.317	464.956	1977.838	-46.959
2300	1065.855	2188.732	1410.193	1790.640	466.601	2046.567	-46.478
2400	1070.641	2234.197	1443.585	1897.469	468.002	2115.176	-46.035
2500	1074.932	2277.992	1476.091	2004.752	469.174	2183.855	-45.628
2600	1078.792	2320.228	1507.750	2112.441	470.080	2252.365	-45.250
2700	1082.275	2361.008	1538.602	2220.497	470.724	2320.926	-44.900
2800	1085.427	2400.426	1568.681	2328.885	471.080	2389.489	-44.576
2900	1088.289	2438.566	1598.023	2437.573	471.116	2457.988	-44.272
3000	1090.893	2475.505	1626.660	2546.534	470.881	2526.521	-43.990
3100	1093.270	2511.314	1654.623	2655.744	470.291	2594.980	-43.724
3200	1095.445	2546.059	1681.940	2765.182	469.392	2663.546	-43.477
3300	1097.439	2579.799	1708.639	2874.827	468.166	2732.188	-43.246
3400	1099.272	2612.588	1734.746	2984.664	466.581	2800.776	-43.028
3500	1100.959	2644.478	1760.285	3094.677	464.643	2869.396	-42.823
3600	1102.517	2675.515	1785.279	3204.852	462.378	2938.174	-42.631
3700	1103.958	2705.743	1809.749	3315.176	459.751	3007.035	-42.451
3800	1105.292	2735.201	1833.717	3425.640	456.734	3075.909	-42.280
3900	1106.531	2763.928	1857.202	3536.231	453.372	3144.809	-42.119
4000	1107.682	2791.958	1880.222	3646.943	449.647	3213.953	-41.969
4100	1108.755	2819.323	1902.794	3757.765	445.522	3283.113	-41.827
4200	1109.755	2846.053	1924.936	3868.691	441.026	3352.369	-41.692
4300	1110.689	2872.177	1946.662	3979.714	436.145	3421.638	-41.564
4400	1111.563	2897.722	1967.988	4090.827	430.888	3491.125	-41.444
4500	1112.382	2922.711	1988.927	4202.025	425.271	3560.796	-41.332
4600	1113.149	2947.168	2009.494	4313.302	419.238	3630.608	-41.226
4700	1113.871	2971.116	2029.700	4424.653	412.806	3700.429	-41.125
4800	1114.549	2994.574	2049.558	4536.074	406.023	3770.508	-41.031
4900	1115.187	3017.561	2069.079	4647.562	398.810	3840.583	-40.940
5000	1115.789	3040.097	2088.275	4759.111	391.269	3911.013	-40.857

3.406. Dibenzo[*b,qr*]naphtho[3,2,1,8-*defg*]chrysene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-61-2
Point Group: C_{2h}

Length: 15.93 Å
Width: 11.62 Å
Breadth: 3.890 Å
L/B Ratio: 1.371

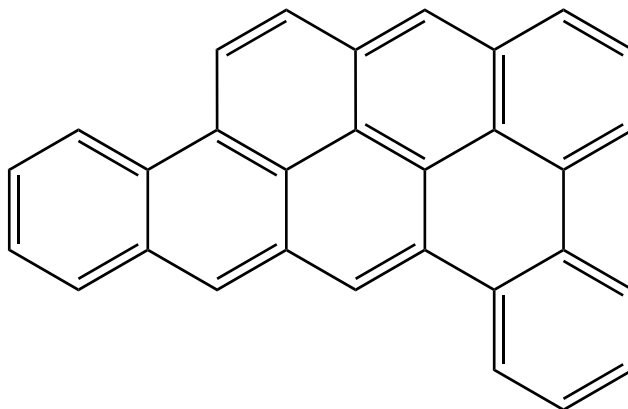
Cartesian coordinates:

C	3.4207	2.5816	0.0000	C	2.7994	1.3436	0.0000	H	0.7031	4.6399	0.0000
C	2.6686	3.7656	0.0000	C	1.3794	1.2769	0.0000	H	-1.3682	3.3457	0.0000
C	1.2946	3.7174	0.0000	C	3.5697	0.1043	0.0000	H	-4.5205	-2.6321	0.0000
C	0.6286	2.4705	0.0000	C	2.9121	-1.1378	0.0000	H	-3.1885	-4.7293	0.0000
C	-0.7929	2.4056	0.0000	C	3.6763	-2.3146	0.0000	H	-0.7031	-4.6399	0.0000
C	-1.4525	1.2029	0.0000	C	5.0595	-2.2649	0.0000	H	1.3682	-3.3457	0.0000
C	-2.7994	-1.3435	0.0000	C	5.7112	-1.0319	0.0000	H	3.1559	-3.2848	0.0000
C	-3.4207	-2.5815	0.0000	C	4.9722	0.1383	0.0000	H	5.6419	-3.1919	0.0000
C	-2.6686	-3.7656	0.0000	C	-3.5696	-0.1043	0.0000	H	6.8052	-0.9906	0.0000
C	-1.2946	-3.7174	0.0000	C	-2.9121	1.1378	0.0000	H	5.4777	1.1164	0.0000
C	-1.3793	-1.2768	0.0000	C	-3.6763	2.3145	0.0000	H	-3.1560	3.2848	0.0000
C	-0.6286	-2.4705	0.0000	C	-5.0595	2.2648	0.0000	H	-5.6420	3.1918	0.0000
C	0.7929	-2.4056	0.0000	C	-5.7112	1.0318	0.0000	H	-6.8051	0.9904	0.0000
C	-0.7000	-0.0195	0.0000	C	-4.9721	-0.1384	0.0000	H	-5.4776	-1.1165	0.0000
C	0.7000	0.0195	0.0000	H	4.5205	2.6321	0.0000				
C	1.4525	-1.2029	0.0000	H	3.1884	4.7294	0.0000				

Table 3.406: Table of thermodynamic data as a function of temperature for Dibenzob[*b,qr*]naphtho[3,2,1,8-*defg*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.964	466.120	466.120	∞
100	116.611	357.875	825.985	-46.811	492.783	540.433	-282.288
200	234.213	472.897	620.624	-29.545	478.717	593.689	-155.052
250	302.143	532.403	596.998	-16.149	472.065	623.200	-130.208
298.15	368.487	591.304	591.304	0.000	466.120	652.862	-114.376
300	371.008	593.592	591.311	0.684	465.900	654.019	-113.872
350	437.398	655.817	596.074	20.910	460.404	685.819	-102.351
400	499.106	718.312	607.449	44.345	455.623	718.346	-93.804
450	555.098	780.389	623.222	70.725	451.475	751.440	-87.223
500	605.193	841.518	642.005	99.756	447.871	784.990	-82.006
600	689.205	959.589	685.183	164.644	441.986	852.996	-74.258
700	755.546	1071.009	732.425	237.009	437.657	921.867	-68.789
800	808.613	1175.489	781.349	315.312	434.706	991.246	-64.720
900	851.730	1273.304	830.636	398.401	432.953	1060.914	-61.573
1000	887.244	1364.939	879.534	485.405	432.235	1130.734	-59.062
1100	916.824	1450.932	927.611	575.652	432.351	1200.595	-57.010
1200	941.683	1531.802	974.625	668.613	433.157	1270.394	-55.298
1300	962.733	1608.031	1020.445	763.862	434.468	1340.117	-53.845
1400	980.676	1680.051	1065.011	861.056	436.150	1409.728	-52.597
1500	996.064	1748.249	1108.308	959.912	438.123	1479.211	-51.510
1600	1009.334	1812.968	1150.344	1060.198	440.251	1548.546	-50.554
1700	1020.838	1874.511	1191.147	1161.720	442.461	1617.719	-49.705
1800	1030.860	1933.151	1230.753	1264.317	444.675	1686.831	-48.950
1900	1039.633	1989.127	1269.206	1367.851	446.863	1755.764	-48.268
2000	1047.347	2042.653	1306.550	1472.208	448.970	1824.611	-47.653
2100	1054.160	2093.922	1342.831	1577.290	450.914	1893.341	-47.093
2200	1060.200	2143.104	1378.097	1683.014	452.696	1961.985	-46.582
2300	1065.577	2190.352	1412.392	1789.308	454.312	2030.552	-46.114
2400	1070.381	2235.806	1445.760	1896.110	455.687	2099.000	-45.683
2500	1074.689	2279.590	1478.243	2003.368	456.834	2167.518	-45.287
2600	1078.564	2321.817	1509.881	2111.034	457.716	2235.869	-44.918
2700	1082.060	2362.589	1540.712	2219.068	458.338	2304.271	-44.578
2800	1085.226	2401.999	1570.773	2327.435	458.673	2372.677	-44.262
2900	1088.099	2440.132	1600.097	2436.103	458.690	2441.019	-43.967
3000	1090.714	2477.065	1628.717	2545.046	458.436	2509.395	-43.692
3100	1093.101	2512.869	1656.663	2654.239	457.829	2577.698	-43.433
3200	1095.285	2547.609	1683.965	2763.660	456.914	2646.109	-43.192
3300	1097.287	2581.343	1710.650	2873.290	455.672	2714.596	-42.968
3400	1099.128	2614.128	1736.743	2983.112	454.072	2783.030	-42.755
3500	1100.823	2646.014	1762.268	3093.110	452.120	2851.496	-42.555
3600	1102.387	2677.048	1787.250	3203.272	449.842	2920.120	-42.369
3700	1103.834	2707.272	1811.709	3313.584	447.202	2988.829	-42.194
3800	1105.174	2736.727	1835.665	3424.035	444.173	3057.550	-42.028
3900	1106.419	2765.451	1859.139	3534.615	440.800	3126.297	-41.871
4000	1107.575	2793.478	1882.149	3645.316	437.064	3195.289	-41.725
4100	1108.652	2820.840	1904.711	3756.128	432.928	3264.298	-41.587
4200	1109.657	2847.568	1926.843	3867.044	428.422	3333.402	-41.456
4300	1110.595	2873.690	1948.560	3978.057	423.531	3402.520	-41.332
4400	1111.473	2899.232	1969.877	4089.161	418.265	3471.855	-41.215
4500	1112.295	2924.219	1990.808	4200.350	412.640	3541.375	-41.106
4600	1113.067	2948.675	2011.367	4311.618	406.599	3611.037	-41.004
4700	1113.791	2972.621	2031.565	4422.962	400.158	3680.707	-40.906
4800	1114.473	2996.077	2051.416	4534.375	393.367	3750.636	-40.814
4900	1115.114	3019.063	2070.930	4645.855	386.147	3820.560	-40.727
5000	1115.719	3041.598	2090.118	4757.397	378.599	3890.840	-40.646

3.407. Anthra[8,9,1,2-*cdefg*]benzo[*a*]naphthacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-82-7
Point Group: C_s

Length: 16.06 Å
Width: 11.38 Å
Breadth: 3.886 Å
L/B Ratio: 1.410

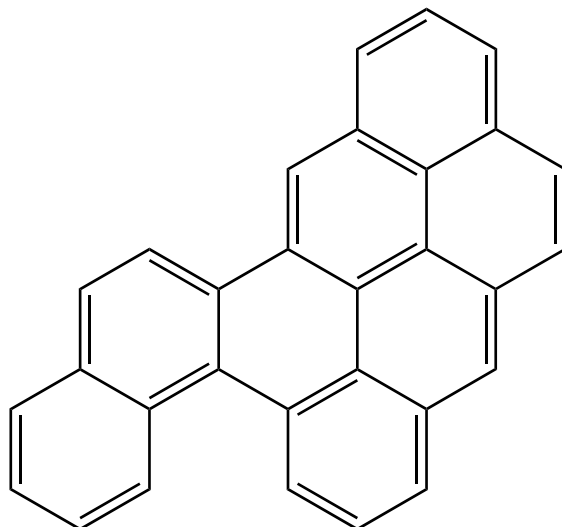
Cartesian coordinates:

C	-6.3599	-0.0024	0.0000	C	0.8370	3.1523	0.0000	H	-5.0011	-3.1362	0.0000
C	-6.2836	-1.4179	0.0000	C	0.9618	0.3345	0.0000	H	-5.2620	1.8498	0.0000
C	-5.0698	-2.0424	0.0000	C	-0.2765	0.9893	0.0000	H	-2.5686	-3.0217	0.0000
C	-5.2206	0.7498	0.0000	C	-0.3315	2.4164	0.0000	H	-0.1171	-2.9281	0.0000
C	-3.9371	0.1310	0.0000	C	-1.6231	3.0591	0.0000	H	5.5661	0.7275	0.0000
C	-3.8630	-1.2815	0.0000	C	-2.7630	2.3339	0.0000	H	5.4408	3.2070	0.0000
C	-2.6089	-1.9254	0.0000	C	-2.7366	0.8936	0.0000	H	3.2361	4.3569	0.0000
C	-1.4374	-1.1863	0.0000	C	-1.4978	0.2383	0.0000	H	0.7996	4.2487	0.0000
C	-0.1529	-1.8264	0.0000	C	3.4961	-1.0074	0.0000	H	-1.6516	4.1548	0.0000
C	1.0079	-1.1091	0.0000	C	2.3135	-1.7675	0.0000	H	-3.7513	2.8192	0.0000
C	3.4368	0.4522	0.0000	C	2.4012	-3.1668	0.0000	H	1.4714	-3.7564	0.0000
C	4.5821	1.2212	0.0000	C	3.6312	-3.8035	0.0000	H	3.6828	-4.8970	0.0000
C	4.5110	2.6287	0.0000	C	4.8033	-3.0495	0.0000	H	5.7771	-3.5498	0.0000
C	3.2976	3.2627	0.0000	C	4.7336	-1.6663	0.0000	H	5.6548	-1.0633	0.0000
C	2.1612	1.0938	0.0000	H	-7.3443	0.4768	0.0000				
C	2.0945	2.5065	0.0000	H	-7.2113	-1.9995	0.0000				

Table 3.407: Table of thermodynamic data as a function of temperature for Anthra[8,9,1,2-*cdefg*]benzo[*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.883	480.956	480.956	∞
100	115.764	360.953	829.164	-46.821	507.609	554.952	-289.871
200	234.380	475.655	623.633	-29.596	493.503	607.923	-158.770
250	302.700	535.246	599.964	-16.180	486.871	637.294	-133.153
298.15	369.180	594.260	594.260	0.000	480.956	666.817	-116.821
300	371.703	596.551	594.267	0.685	480.738	667.968	-116.301
350	438.074	658.884	599.038	20.946	475.276	699.618	-104.410
400	499.694	721.463	610.431	44.413	470.527	731.989	-95.586
450	555.583	783.604	626.227	70.819	466.406	764.924	-88.788
500	605.584	844.779	645.033	99.873	462.823	798.312	-83.397
600	689.463	962.908	688.255	164.792	456.970	865.989	-75.389
700	755.734	1074.362	735.535	237.179	452.663	934.526	-69.734
800	808.770	1178.865	784.491	315.499	449.729	1003.568	-65.525
900	851.874	1276.697	833.805	398.603	447.991	1072.898	-62.268
1000	887.384	1368.348	882.726	485.621	447.288	1142.378	-59.670
1100	916.962	1454.353	930.824	575.882	447.417	1211.898	-57.547
1200	941.819	1535.236	977.855	668.857	448.237	1281.354	-55.775
1300	962.866	1611.475	1023.691	764.119	449.562	1350.733	-54.272
1400	980.806	1683.505	1068.272	861.326	451.257	1419.999	-52.980
1500	996.189	1751.712	1111.582	960.195	453.242	1489.136	-51.855
1600	1009.453	1816.438	1153.630	1060.494	455.382	1558.124	-50.866
1700	1020.951	1877.989	1194.444	1162.027	457.604	1626.950	-49.989
1800	1030.968	1936.635	1234.060	1264.634	459.829	1695.714	-49.207
1900	1039.736	1992.617	1272.522	1368.179	462.028	1764.298	-48.503
2000	1047.444	2046.148	1309.875	1472.546	464.145	1832.796	-47.867
2100	1054.252	2097.421	1346.165	1577.638	466.098	1901.177	-47.288
2200	1060.287	2146.607	1381.439	1683.371	467.889	1969.470	-46.760
2300	1065.659	2193.860	1415.741	1789.673	469.514	2037.687	-46.276
2400	1070.459	2239.317	1449.115	1896.484	470.896	2105.783	-45.830
2500	1074.762	2283.104	1481.605	2003.749	472.051	2173.951	-45.421
2600	1078.633	2325.334	1513.249	2111.422	472.940	2241.949	-45.040
2700	1082.126	2366.108	1544.085	2219.463	473.569	2310.000	-44.689
2800	1085.288	2405.521	1574.151	2327.836	473.910	2378.054	-44.362
2900	1088.158	2443.656	1603.480	2436.511	473.933	2446.043	-44.057
3000	1090.770	2480.591	1632.105	2545.459	473.685	2514.067	-43.773
3100	1093.154	2516.397	1660.056	2654.657	473.083	2582.018	-43.506
3200	1095.335	2551.138	1687.362	2764.083	472.174	2650.075	-43.257
3300	1097.335	2584.874	1714.050	2873.718	470.936	2718.210	-43.025
3400	1099.173	2617.660	1740.147	2983.545	469.341	2786.290	-42.805
3500	1100.866	2649.547	1765.677	3093.548	467.394	2854.403	-42.599
3600	1102.429	2680.582	1790.662	3203.714	465.120	2922.674	-42.406
3700	1103.874	2710.807	1815.124	3314.030	462.484	2991.029	-42.225
3800	1105.212	2740.264	1839.084	3424.485	459.459	3059.397	-42.053
3900	1106.455	2768.989	1862.561	3535.069	456.089	3127.790	-41.891
4000	1107.610	2797.016	1885.573	3645.773	452.357	3196.428	-41.740
4100	1108.685	2824.379	1908.138	3756.588	448.225	3265.083	-41.597
4200	1109.689	2851.108	1930.273	3867.508	443.722	3333.834	-41.461
4300	1110.626	2877.231	1951.993	3978.524	438.834	3402.597	-41.333
4400	1111.502	2902.774	1973.312	4089.631	433.571	3471.579	-41.212
4500	1112.324	2927.762	1994.246	4200.823	427.949	3540.744	-41.099
4600	1113.094	2952.218	2014.806	4312.094	421.910	3610.051	-40.993
4700	1113.817	2976.164	2035.007	4423.440	415.472	3679.368	-40.891
4800	1114.497	2999.621	2054.859	4534.856	408.684	3748.942	-40.796
4900	1115.138	3022.608	2074.375	4646.338	401.466	3818.512	-40.705
5000	1115.742	3045.143	2093.566	4757.882	393.921	3888.437	-40.621

3.408. Benzo[*de*]naphtho[8,1,2,3-*stuv*]picene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-74-7
Point Group: C₁

Length: 16.03 Å
Width: 11.15 Å
Breadth: 5.003 Å
L/B Ratio: 1.438

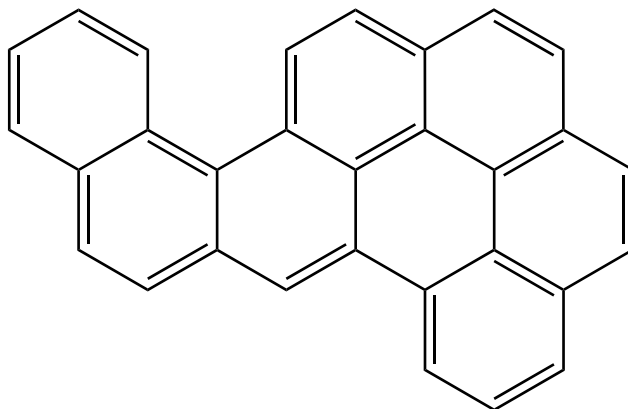
Cartesian coordinates:

C	5.2429	-2.0537	0.0700	C	-2.6072	-1.8537	-0.0710	H	-2.2352	3.9884	0.1234
C	3.8674	-1.7427	-0.0939	C	-1.2039	-2.0518	-0.2112	H	-0.0056	4.8726	-0.2776
C	3.4000	-0.4243	0.1037	C	-4.5035	-0.3280	0.2184	H	2.4130	4.4839	-0.7195
C	4.3399	0.5242	0.5921	C	-5.3654	-1.4145	0.2200	H	3.3485	2.2225	-0.6770
C	5.6580	0.2016	0.7793	C	-4.8631	-2.7150	0.0756	H	-3.1243	-3.9573	-0.1827
C	6.1263	-1.0967	0.4899	C	-3.5105	-2.9381	-0.0691	H	-5.5597	-3.5601	0.0780
C	2.0074	-0.1265	-0.1220	C	-2.7147	1.8940	0.1627	H	-6.4442	-1.2591	0.3332
C	1.1220	-1.1937	-0.2588	C	-4.1416	2.0783	0.3294	H	-0.8306	-3.0817	-0.3279
C	1.6157	-2.5164	-0.4389	C	-4.9870	1.0287	0.3577	H	3.3298	-3.7914	-0.6008
C	2.9504	-2.7803	-0.4140	C	-0.4574	2.7548	-0.0968	H	0.8924	-3.3278	-0.6125
C	1.4800	1.2373	-0.2203	C	-1.8543	2.9607	0.0739	H	4.0014	1.5393	0.8407
C	0.0716	1.4443	-0.1073	C	2.2726	2.3415	-0.4891	H	6.3605	0.9495	1.1619
C	-0.8255	0.3395	-0.0603	C	1.7423	3.6415	-0.5193	H	7.1880	-1.3291	0.6201
C	-0.3240	-0.9972	-0.1939	C	0.4068	3.8574	-0.2900	H	5.5806	-3.0765	-0.1336
C	-2.2028	0.5597	0.0642	H	-6.0661	1.1743	0.4838				
C	-3.1068	-0.5429	0.0737	H	-4.5121	3.1050	0.4304				

Table 3.408: Table of thermodynamic data as a function of temperature for Benzo[de]naphtho[8,1,2,3-stuv]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.466	495.571	495.571	∞
100	113.425	354.683	821.132	-46.645	522.400	570.369	-297.924
200	233.611	468.275	616.128	-29.570	508.142	624.038	-162.979
250	302.478	527.756	592.470	-16.179	501.486	653.782	-136.597
298.15	369.334	586.765	586.765	0.000	495.571	683.666	-119.773
300	371.869	589.058	586.772	0.686	495.352	684.831	-119.237
350	438.501	651.437	591.547	20.962	489.906	716.854	-106.982
400	500.286	714.085	602.950	44.454	485.183	749.596	-97.885
450	556.269	776.302	618.761	70.893	481.094	782.898	-90.875
500	606.317	837.552	637.588	99.982	477.547	816.649	-85.313
600	690.203	955.817	680.857	164.976	471.768	885.042	-77.048
700	756.428	1067.381	728.189	237.434	467.533	954.283	-71.208
800	809.402	1171.973	777.197	315.821	464.666	1024.018	-66.860
900	852.443	1269.876	826.560	398.985	462.988	1094.033	-63.495
1000	887.894	1361.584	875.526	486.057	462.338	1164.192	-60.810
1100	917.419	1447.635	923.666	576.367	462.515	1234.386	-58.615
1200	942.229	1528.555	970.735	669.384	463.379	1304.512	-56.783
1300	963.235	1604.826	1016.606	764.686	464.743	1374.558	-55.229
1400	981.139	1676.882	1061.219	861.928	466.473	1444.487	-53.893
1500	996.490	1745.111	1104.558	960.829	468.489	1514.285	-52.731
1600	1009.727	1809.856	1146.633	1061.156	470.658	1583.933	-51.709
1700	1021.201	1871.422	1187.472	1162.715	472.906	1653.416	-50.802
1800	1031.196	1930.082	1227.112	1265.347	475.155	1722.836	-49.994
1900	1039.944	1986.075	1265.595	1368.913	477.376	1792.075	-49.267
2000	1047.636	2039.617	1302.967	1473.300	479.513	1861.227	-48.609
2100	1054.428	2090.899	1339.275	1578.410	481.485	1930.260	-48.012
2200	1060.451	2140.093	1374.566	1684.160	483.293	1999.205	-47.466
2300	1065.811	2187.352	1408.884	1790.478	484.933	2068.073	-46.966
2400	1070.600	2232.816	1442.273	1897.303	486.330	2136.820	-46.506
2500	1074.893	2276.609	1474.776	2004.582	487.499	2205.637	-46.083
2600	1078.755	2318.843	1506.433	2112.268	488.400	2274.285	-45.690
2700	1082.240	2359.622	1537.281	2220.320	489.041	2342.984	-45.327
2800	1085.395	2399.039	1567.359	2328.705	489.393	2411.686	-44.990
2900	1088.258	2437.177	1596.698	2437.390	489.426	2480.324	-44.675
3000	1090.865	2474.116	1625.333	2546.348	489.188	2548.995	-44.381
3100	1093.243	2509.924	1653.294	2655.555	488.596	2617.594	-44.105
3200	1095.419	2544.668	1680.609	2764.990	487.694	2686.298	-43.848
3300	1097.414	2578.407	1707.306	2874.633	486.465	2755.080	-43.608
3400	1099.248	2611.196	1733.411	2984.467	484.878	2823.807	-43.382
3500	1100.937	2643.085	1758.949	3094.477	482.938	2892.566	-43.168
3600	1102.496	2674.121	1783.941	3204.650	480.671	2961.483	-42.969
3700	1103.937	2704.349	1808.410	3314.973	478.041	3030.484	-42.782
3800	1105.273	2733.807	1832.377	3425.434	475.023	3099.498	-42.605
3900	1106.512	2762.533	1855.860	3536.024	471.659	3168.537	-42.437
4000	1107.665	2790.562	1878.879	3646.734	467.932	3237.820	-42.281
4100	1108.738	2817.927	1901.450	3757.554	463.805	3307.120	-42.132
4200	1109.739	2844.657	1923.590	3868.479	459.308	3376.516	-41.992
4300	1110.674	2870.780	1945.315	3979.500	454.425	3445.925	-41.859
4400	1111.548	2896.324	1966.640	4090.612	449.166	3515.551	-41.734
4500	1112.367	2921.313	1987.578	4201.808	443.548	3585.362	-41.617
4600	1113.136	2945.770	2008.144	4313.083	437.514	3655.314	-41.507
4700	1113.858	2969.718	2028.349	4424.433	431.080	3725.275	-41.401
4800	1114.536	2993.175	2048.206	4535.853	424.296	3795.494	-41.303
4900	1115.175	3016.163	2067.726	4647.339	417.082	3865.708	-41.208
5000	1115.778	3038.698	2086.921	4758.887	409.540	3936.278	-41.121

3.409. Benzo[ghi]naphtho[2,1-b]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-63-4
Point Group: C₁

Length: 16.22 Å
Width: 11.10 Å
Breadth: 4.931 Å
L/B Ratio: 1.461

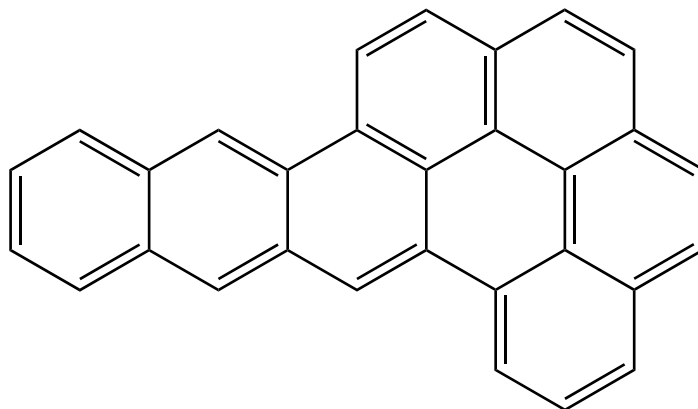
Cartesian coordinates:

C	3.4227	3.0413	0.0704	C	1.3062	1.1815	0.1219	H	6.3520	-0.5013	-0.3646
C	2.1357	3.4788	0.2127	C	1.0574	2.5546	0.2442	H	5.8580	1.9272	-0.2061
C	3.7044	1.6530	-0.0349	C	-0.2872	2.9941	0.4201	H	1.3659	-3.7091	-0.0446
C	5.3219	-0.1420	-0.2584	C	-1.3157	2.1054	0.3939	H	3.7210	-4.4784	-0.2757
C	5.0517	1.1856	-0.1722	C	-1.8808	-1.5988	0.2448	H	5.5783	-2.8291	-0.3833
C	4.2666	-1.1114	-0.2106	C	-2.1956	-0.2364	0.1063	H	-0.3229	-3.1241	0.2553
C	2.1837	-2.9738	-0.0961	C	-4.2141	-2.2187	0.4368	H	-0.4733	4.0615	0.5861
C	3.5096	-3.4052	-0.2233	C	-2.9100	-2.5790	0.4384	H	-2.3379	2.4722	0.5601
C	4.5405	-2.4920	-0.2822	C	-4.5835	-0.8708	0.1213	H	-5.0067	-2.9493	0.6349
C	2.9336	-0.6741	-0.0845	C	-3.5908	0.1067	-0.1044	H	-2.6124	-3.6200	0.6103
C	2.6537	0.7287	-0.0011	C	-4.0212	1.3569	-0.6079	H	-3.2771	2.1149	-0.8877
C	1.8803	-1.6211	-0.0296	C	-5.3550	1.6466	-0.7769	H	-5.6597	2.6225	-1.1694
C	0.5025	-1.1539	0.0914	C	-6.3360	0.6957	-0.4541	H	-7.3955	0.9474	-0.5655
C	-0.5381	-2.0436	0.2099	C	-5.9524	-0.5512	-0.0233	H	-6.7042	-1.3171	0.2003
C	-1.1113	0.7039	0.1833	H	4.2552	3.7534	0.0390				
C	0.2197	0.2460	0.1234	H	1.9153	4.5487	0.3028				

Table 3.409: Table of thermodynamic data as a function of temperature for Benzo[ghi]naphtho[2,1-b]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.431	471.662	471.662	∞
100	113.373	356.786	822.263	-46.548	498.588	546.347	-285.376
200	233.083	470.122	617.685	-29.513	484.291	599.818	-156.653
250	301.885	529.478	594.073	-16.149	477.607	629.472	-131.518
298.15	368.696	588.378	588.378	0.000	471.662	659.276	-115.500
300	371.230	590.667	588.386	0.684	471.442	660.438	-114.990
350	437.844	652.946	593.152	20.928	465.964	692.383	-103.330
400	499.638	715.507	604.537	44.388	461.208	725.052	-94.680
450	555.648	777.648	620.326	70.795	457.087	758.285	-88.018
500	605.732	838.835	639.127	99.854	453.509	791.970	-82.735
600	689.703	957.000	682.346	164.793	447.677	860.240	-74.889
700	756.010	1068.494	729.629	237.206	443.396	929.366	-69.349
800	809.055	1173.035	778.592	315.554	440.490	998.993	-65.226
900	852.156	1270.901	827.916	398.687	438.780	1068.903	-62.036
1000	887.655	1362.580	876.848	485.733	438.104	1138.962	-59.492
1100	917.218	1448.611	924.957	576.020	438.260	1209.057	-57.412
1200	942.060	1529.515	971.999	669.019	439.105	1279.086	-55.676
1300	963.091	1605.774	1017.847	764.305	440.453	1349.036	-54.204
1400	981.015	1677.820	1062.438	861.534	442.170	1418.872	-52.938
1500	996.383	1746.040	1105.758	960.423	444.175	1488.577	-51.836
1600	1009.634	1810.779	1147.816	1060.740	446.334	1558.131	-50.867
1700	1021.119	1872.340	1188.639	1162.291	448.573	1627.523	-50.007
1800	1031.123	1930.995	1228.265	1264.915	450.814	1696.851	-49.240
1900	1039.880	1986.985	1266.735	1368.474	453.028	1765.998	-48.550
2000	1047.579	2040.524	1304.096	1472.855	455.159	1835.060	-47.926
2100	1054.377	2091.803	1340.394	1577.960	457.126	1904.002	-47.358
2200	1060.404	2140.995	1375.674	1683.705	458.929	1972.857	-46.841
2300	1065.768	2188.252	1409.983	1790.019	460.564	2041.635	-46.366
2400	1070.561	2233.714	1443.364	1896.840	461.957	2110.292	-45.928
2500	1074.858	2277.505	1475.859	2004.114	463.122	2179.020	-45.527
2600	1078.722	2319.738	1507.509	2111.797	464.020	2247.578	-45.153
2700	1082.210	2360.516	1538.351	2219.846	464.658	2316.188	-44.808
2800	1085.367	2399.932	1568.422	2328.228	465.007	2384.801	-44.488
2900	1088.232	2438.069	1597.756	2436.910	465.038	2453.349	-44.189
3000	1090.840	2475.007	1626.385	2545.866	464.797	2521.931	-43.910
3100	1093.221	2510.815	1654.340	2655.071	464.202	2590.441	-43.648
3200	1095.398	2545.558	1681.651	2764.503	463.299	2659.056	-43.404
3300	1097.395	2579.296	1708.343	2874.144	462.068	2727.749	-43.176
3400	1099.230	2612.084	1734.444	2983.977	460.478	2796.387	-42.960
3500	1100.920	2643.973	1759.977	3093.985	458.537	2865.057	-42.758
3600	1102.480	2675.009	1784.965	3204.156	456.268	2933.886	-42.569
3700	1103.922	2705.236	1809.431	3314.477	453.637	3002.798	-42.391
3800	1105.258	2734.693	1833.394	3424.937	450.617	3071.723	-42.223
3900	1106.499	2763.419	1856.874	3535.526	447.251	3140.673	-42.064
4000	1107.652	2791.448	1879.889	3646.234	443.524	3209.868	-41.916
4100	1108.725	2818.812	1902.458	3757.053	439.395	3279.079	-41.775
4200	1109.727	2845.542	1924.595	3867.977	434.896	3348.387	-41.642
4300	1110.662	2871.665	1946.317	3978.997	430.012	3417.707	-41.516
4400	1111.537	2897.209	1967.639	4090.107	424.753	3487.245	-41.398
4500	1112.357	2922.198	1988.575	4201.302	419.134	3556.967	-41.287
4600	1113.126	2946.655	2009.138	4312.577	413.098	3626.830	-41.183
4700	1113.848	2970.602	2029.341	4423.926	406.664	3696.703	-41.083
4800	1114.527	2994.059	2049.196	4535.345	399.879	3766.833	-40.991
4900	1115.167	3017.046	2068.714	4646.830	392.664	3836.960	-40.902
5000	1115.769	3039.582	2087.907	4758.377	385.121	3907.441	-40.820

3.410. Benzo[uv]naphtho[2,1,8,7-defg]pentacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 5869-31-8
Point Group: C_s

Length: 16.73 Å
Width: 11.37 Å
Breadth: 3.886 Å
L/B Ratio: 1.472

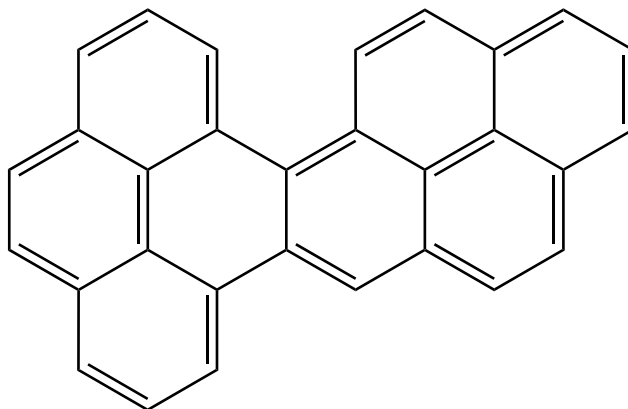
Cartesian coordinates:

C	0.7584	1.6007	0.0000	C	-1.7040	1.6557	0.0000	H	1.6819	-3.1860	0.0000
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C	-0.4623	-3.3266	0.0000	C	-2.9230	-0.5042	0.0000	H	-2.9294	-4.4104	0.0000
C	0.7215	-2.6476	0.0000	C	-1.6840	-1.2165	0.0000	H	-6.3206	1.4320	0.0000
C	-1.6961	-2.6201	0.0000	C	2.0110	0.9036	0.0000	H	-6.3038	-1.0514	0.0000
C	-4.1200	-2.6295	0.0000	C	2.0198	-0.5191	0.0000	H	-0.7996	3.6060	0.0000
C	-2.9408	-3.3144	0.0000	C	3.2371	-1.1933	0.0000	H	-2.9695	4.8202	0.0000
C	-4.1318	-1.2051	0.0000	C	3.2130	1.6072	0.0000	H	-5.1148	3.5625	0.0000
C	-5.3760	0.8761	0.0000	C	4.4382	0.9267	0.0000	H	3.2403	-2.2952	0.0000
C	-5.3669	-0.4824	0.0000	C	4.4501	-0.4912	0.0000	H	3.2047	2.7042	0.0000
C	-4.1511	1.6189	0.0000	C	5.7061	-1.1753	0.0000	H	5.7055	-2.2711	0.0000
C	-1.7448	3.0414	0.0000	C	6.8734	-0.4734	0.0000	H	7.8378	-0.9919	0.0000
C	-2.9687	3.7251	0.0000	C	6.8616	0.9493	0.0000	H	7.8172	1.4836	0.0000
C	-4.1569	3.0303	0.0000	C	5.6828	1.6316	0.0000	H	5.6640	2.7273	0.0000
C	-0.4440	-0.5104	0.0000	H	0.7670	2.7032	0.0000				
C	-0.4321	0.9339	0.0000	H	-0.4796	-4.4224	0.0000				

Table 3.410: Table of thermodynamic data as a function of temperature for Benzo[uv]naphtho[2,1,8,7-defg]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.520	462.219	462.219	∞
100	113.959	357.754	823.781	-46.603	489.090	536.753	-280.365
200	233.327	471.382	619.020	-29.528	474.834	590.108	-154.117
250	302.038	530.782	595.398	-16.154	468.159	619.699	-129.476
298.15	368.754	589.702	589.702	0.000	462.219	649.439	-113.777
300	371.284	591.991	589.709	0.685	462.000	650.599	-113.277
350	437.788	654.270	594.475	20.928	456.521	682.478	-101.852
400	499.479	716.816	605.860	44.382	451.760	715.080	-93.378
450	555.408	778.934	621.646	70.779	447.629	748.249	-86.853
500	605.438	840.092	640.443	99.825	444.038	781.870	-81.680
600	689.367	958.199	683.646	164.732	438.173	850.017	-73.999
700	755.691	1069.642	730.911	237.112	433.859	919.026	-68.577
800	808.776	1174.143	779.855	315.430	430.923	988.540	-64.544
900	851.923	1271.979	829.160	398.537	429.188	1058.342	-61.423
1000	887.467	1363.636	878.074	485.562	428.491	1128.293	-58.935
1100	917.068	1449.650	926.166	575.833	428.630	1198.284	-56.901
1200	941.941	1530.543	973.194	668.818	429.462	1268.210	-55.203
1300	962.998	1606.793	1019.028	764.094	430.799	1338.058	-53.763
1400	980.942	1678.833	1063.608	861.314	432.508	1407.791	-52.524
1500	996.326	1747.049	1106.917	960.197	434.506	1477.395	-51.446
1600	1009.589	1811.784	1148.966	1060.509	436.660	1546.849	-50.498
1700	1021.084	1873.343	1189.780	1162.056	438.895	1616.140	-49.657
1800	1031.097	1931.996	1229.398	1264.676	441.134	1685.369	-48.907
1900	1039.859	1987.985	1267.862	1368.234	443.345	1754.416	-48.231
2000	1047.563	2041.523	1305.216	1472.613	445.474	1823.377	-47.621
2100	1054.364	2092.801	1341.508	1577.716	447.440	1892.220	-47.065
2200	1060.395	2141.992	1376.783	1683.460	449.241	1960.975	-46.559
2300	1065.762	2189.249	1411.087	1789.773	450.876	2029.653	-46.094
2400	1070.556	2234.711	1444.464	1896.593	452.269	2098.210	-45.665
2500	1074.855	2278.502	1476.955	2003.868	453.433	2166.838	-45.273
2600	1078.721	2320.735	1508.601	2111.550	454.331	2235.297	-44.907
2700	1082.209	2361.513	1539.439	2219.599	454.969	2303.807	-44.569
2800	1085.367	2400.928	1569.507	2327.981	455.318	2372.320	-44.255
2900	1088.233	2439.066	1598.837	2436.663	455.348	2440.769	-43.962
3000	1090.842	2476.004	1627.464	2545.619	455.108	2509.251	-43.689
3100	1093.222	2511.811	1655.417	2654.824	454.513	2577.661	-43.432
3200	1095.400	2546.555	1682.725	2764.257	453.610	2646.177	-43.194
3300	1097.397	2580.293	1709.415	2873.898	452.379	2714.770	-42.970
3400	1099.232	2613.081	1735.513	2983.731	450.790	2783.308	-42.759
3500	1100.922	2644.970	1761.044	3093.739	448.849	2851.879	-42.561
3600	1102.482	2676.006	1786.031	3203.911	446.580	2920.608	-42.376
3700	1103.925	2706.233	1810.495	3314.232	443.949	2989.420	-42.202
3800	1105.261	2735.691	1834.456	3424.692	440.929	3058.245	-42.038
3900	1106.501	2764.417	1857.934	3535.281	437.564	3127.096	-41.882
4000	1107.655	2792.445	1880.948	3645.989	433.837	3196.191	-41.737
4100	1108.728	2819.810	1903.515	3756.809	429.708	3265.303	-41.600
4200	1109.730	2846.539	1925.651	3867.733	425.210	3334.510	-41.470
4300	1110.665	2872.663	1947.372	3978.753	420.326	3403.731	-41.346
4400	1111.540	2898.207	1968.692	4089.864	415.067	3473.169	-41.231
4500	1112.360	2923.196	1989.627	4201.059	409.448	3542.791	-41.123
4600	1113.129	2947.653	2010.189	4312.334	403.413	3612.555	-41.021
4700	1113.851	2971.600	2030.390	4423.683	396.979	3682.328	-40.924
4800	1114.530	2995.057	2050.244	4535.103	390.194	3752.358	-40.833
4900	1115.169	3018.045	2069.761	4646.588	382.979	3822.385	-40.746
5000	1115.772	3040.580	2088.953	4758.135	375.437	3892.766	-40.667

3.411. Benzo[*pqr*]naphtho[2,1,8-*def*]picene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 100684-90-0
Point Group: C₁

Length: 16.12 Å
Width: 11.06 Å
Breadth: 4.995 Å
L/B Ratio: 1.457

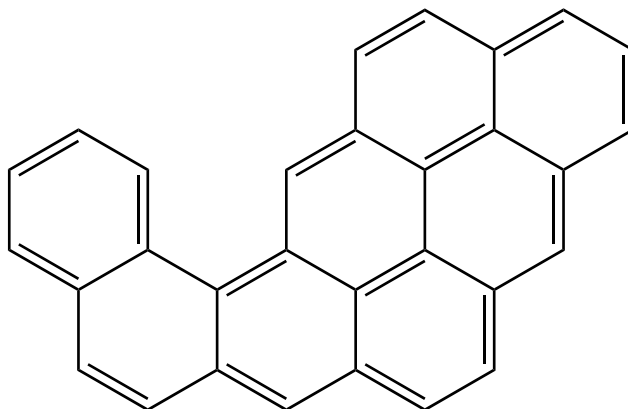
Cartesian coordinates:

C	5.1056	-1.3075	-0.1467	C	-0.4208	2.0484	0.2558	H	0.1358	-2.9440	0.8097
C	5.3836	0.0026	-0.3335	C	-1.7597	1.6864	0.2715	H	1.9947	-4.5334	0.9406
C	3.7572	-1.7515	0.0896	C	-2.7972	2.6665	0.4812	H	4.3190	-3.8203	0.4113
C	1.1480	-2.5848	0.5786	C	-4.1019	2.3208	0.4353	H	5.6718	2.6768	-0.5259
C	2.2018	-3.4954	0.6593	C	-4.4961	0.9624	0.1547	H	3.8525	4.3604	-0.3383
C	3.4951	-3.0985	0.3821	C	-5.8416	0.5979	0.0821	H	1.5069	3.6424	0.0040
C	4.3380	0.9888	-0.2783	C	-6.1997	-0.7157	-0.2069	H	-0.1428	3.1107	0.3480
C	4.6346	2.3568	-0.3757	C	-5.2280	-1.6792	-0.4343	H	-2.4924	3.7001	0.6820
C	3.6214	3.2921	-0.2712	C	-3.4947	-0.0151	-0.0571	H	-4.8916	3.0621	0.6025
C	2.3014	2.8856	-0.0811	C	-3.8717	-1.3394	-0.3646	H	-6.6183	1.3521	0.2525
C	2.6969	-0.8220	0.0501	C	-2.8351	-2.2993	-0.6209	H	-7.2590	-0.9887	-0.2589
C	3.0025	0.5729	-0.0977	C	-1.5293	-1.9662	-0.4986	H	-5.5163	-2.7096	-0.6710
C	1.9714	1.5337	-0.0041	C	-1.0982	-0.6470	-0.1078	H	-3.1308	-3.3088	-0.9296
C	1.3548	-1.2552	0.2138	C	-2.1061	0.3344	0.0364	H	-0.7624	-2.7199	-0.7249
C	0.2652	-0.2880	0.0717	H	5.9000	-2.0625	-0.1664				
C	0.5885	1.0858	0.1230	H	6.4088	0.3448	-0.5158				

Table 3.411: Table of thermodynamic data as a function of temperature for Benzo[*pqr*]naphtho[2,1,8-*def*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.400	481.062	481.062	∞
100	112.794	357.418	822.749	-46.533	508.003	555.699	-290.261
200	233.053	470.499	618.157	-29.532	493.672	609.124	-159.084
250	302.100	529.876	594.527	-16.163	486.993	638.759	-133.459
298.15	369.042	588.827	588.827	0.000	481.062	668.542	-117.123
300	371.579	591.118	588.834	0.685	480.843	669.704	-116.603
350	438.250	653.456	593.605	20.948	475.384	701.625	-104.710
400	500.054	716.072	605.001	44.428	470.648	734.267	-95.883
450	556.051	778.261	620.804	70.856	466.548	767.470	-89.084
500	606.111	839.489	639.621	99.934	462.990	801.123	-83.691
600	690.022	957.719	682.871	164.908	457.192	869.325	-75.680
700	756.273	1069.258	730.185	237.351	452.940	938.377	-70.021
800	809.271	1173.830	779.177	315.723	450.058	1007.925	-65.809
900	852.332	1271.719	828.525	398.875	448.368	1077.755	-62.550
1000	887.800	1363.416	877.479	485.937	447.709	1147.731	-59.950
1100	917.339	1449.459	925.607	576.237	447.877	1217.742	-57.825
1200	942.161	1530.373	972.667	669.248	448.733	1287.686	-56.050
1300	963.176	1606.639	1018.529	764.543	450.091	1357.550	-54.546
1400	981.088	1678.691	1063.134	861.780	451.815	1427.298	-53.252
1500	996.446	1746.916	1106.465	960.676	453.827	1496.916	-52.126
1600	1009.688	1811.658	1148.534	1060.998	455.992	1566.383	-51.136
1700	1021.166	1873.222	1189.367	1162.555	458.236	1635.686	-50.257
1800	1031.165	1931.880	1229.001	1265.182	460.482	1704.926	-49.475
1900	1039.917	1987.872	1267.479	1368.746	462.700	1773.985	-48.769
2000	1047.612	2041.413	1304.847	1473.131	464.834	1842.957	-48.132
2100	1054.406	2092.694	1341.151	1578.238	466.804	1911.811	-47.553
2200	1060.430	2141.886	1376.438	1683.986	468.610	1980.577	-47.024
2300	1065.793	2189.145	1410.753	1790.302	470.248	2049.265	-46.539
2400	1070.583	2234.608	1444.139	1897.126	471.644	2117.833	-46.092
2500	1074.878	2278.400	1476.639	2004.403	472.810	2186.471	-45.683
2600	1078.741	2320.634	1508.293	2112.087	473.711	2254.940	-45.301
2700	1082.227	2361.412	1539.139	2220.138	474.350	2323.461	-44.949
2800	1085.383	2400.828	1569.214	2328.521	474.701	2391.984	-44.622
2900	1088.247	2438.967	1598.551	2437.205	474.733	2460.442	-44.316
3000	1090.854	2475.904	1627.184	2546.162	474.494	2528.935	-44.032
3100	1093.233	2511.713	1655.142	2655.368	473.900	2597.354	-43.764
3200	1095.410	2546.456	1682.456	2764.802	472.998	2665.880	-43.515
3300	1097.406	2580.195	1709.151	2874.444	471.768	2734.483	-43.282
3400	1099.240	2612.983	1735.255	2984.278	470.180	2803.031	-43.062
3500	1100.930	2644.872	1760.790	3094.287	468.239	2871.611	-42.856
3600	1102.489	2675.909	1785.781	3204.459	465.971	2940.350	-42.662
3700	1103.931	2706.136	1810.249	3314.781	463.341	3009.172	-42.481
3800	1105.267	2735.593	1834.214	3425.242	460.322	3078.007	-42.309
3900	1106.506	2764.319	1857.696	3535.831	456.957	3146.867	-42.147
4000	1107.659	2792.349	1880.713	3646.540	453.230	3215.972	-41.995
4100	1108.732	2819.713	1903.283	3757.360	449.102	3285.093	-41.852
4200	1109.734	2846.443	1925.423	3868.284	444.604	3354.311	-41.716
4300	1110.669	2872.566	1947.147	3979.305	439.721	3423.541	-41.587
4400	1111.543	2898.110	1968.470	4090.416	434.462	3492.989	-41.466
4500	1112.363	2923.099	1989.408	4201.612	428.844	3562.621	-41.353
4600	1113.132	2947.556	2009.972	4312.887	422.809	3632.394	-41.246
4700	1113.853	2971.503	2030.176	4424.237	416.374	3702.176	-41.144
4800	1114.532	2994.961	2050.032	4535.656	409.590	3772.217	-41.049
4900	1115.171	3017.948	2069.552	4647.142	402.376	3842.253	-40.958
5000	1115.774	3040.484	2088.746	4758.689	394.833	3912.644	-40.874

3.412. Benzo[*a*]naphtho[7,8,1,2,3-*pqrst*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-78-1
Point Group: C₁

Length: 16.27 Å
Width: 10.96 Å
Breadth: 4.983 Å
L/B Ratio: 1.485

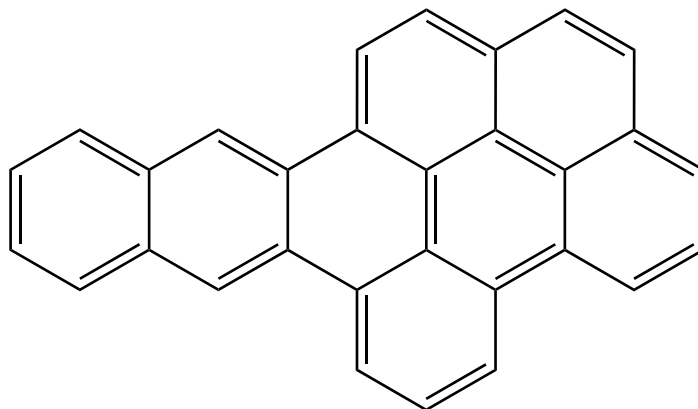
Cartesian coordinates:

C	3.1102	1.9642	-0.6219	C	-1.7393	-3.4066	-0.3019	H	-6.2478	-1.1228	-0.3468
C	3.3702	0.6686	-0.1137	C	-0.4142	-3.6229	-0.2128	H	-4.3358	-2.6837	-0.3992
C	4.7166	0.3455	0.1611	C	-1.8836	0.3304	0.0734	H	-2.4419	-4.2371	-0.4368
C	5.7271	1.3292	0.0590	C	-3.2911	0.5589	0.0340	H	-0.0017	-4.6372	-0.2670
C	5.4258	2.5958	-0.3776	C	-4.1730	-0.5279	-0.1492	H	2.2475	-3.7842	0.1778
C	4.1062	2.9032	-0.7480	C	-3.6393	-1.8464	-0.2680	H	1.0431	2.0500	0.4589
C	5.0853	-0.9989	0.4862	C	-3.8028	1.8740	0.1833	H	-0.8420	3.5736	0.6088
C	4.1552	-1.9819	0.4490	C	-5.1748	2.0821	0.1301	H	-3.2868	3.9677	0.5219
C	2.7766	-1.6753	0.2039	C	-6.0445	1.0028	-0.0646	H	4.4335	-3.0272	0.6277
C	2.3480	-0.3465	0.0557	C	-5.5597	-0.2827	-0.1999	H	6.1329	-1.2161	0.7240
C	1.8624	-2.7581	0.1224	C	-0.9862	1.4207	0.2662	H	6.7576	1.0616	0.3199
C	0.5212	-2.5283	-0.0461	C	0.3739	1.1963	0.2781	H	6.2050	3.3604	-0.4580
C	0.0311	-1.1843	-0.0174	C	-2.8725	2.9608	0.3957	H	3.8769	3.8980	-1.1442
C	0.9277	-0.0951	0.0834	C	-1.5411	2.7460	0.4414	H	2.0933	2.2276	-0.9428
C	-1.3740	-0.9674	-0.0543	H	-5.5808	3.0937	0.2424				
C	-2.2874	-2.0678	-0.2122	H	-7.1234	1.1865	-0.1062				

Table 3.412: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[7,8,1,2,3-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.512	490.595	490.595	∞
100	112.983	355.501	822.293	-46.679	517.390	565.277	-295.265
200	233.857	468.929	617.049	-29.624	503.113	618.878	-161.631
250	303.055	528.504	593.347	-16.211	496.478	648.587	-135.512
298.15	370.070	587.630	587.630	0.000	490.595	678.432	-118.856
300	372.609	589.927	587.637	0.687	490.378	679.596	-118.326
350	439.289	652.425	592.421	21.002	484.971	711.573	-106.194
400	501.059	715.178	603.845	44.533	480.286	744.262	-97.189
450	556.999	777.483	619.684	71.010	476.235	777.508	-90.249
500	606.994	838.808	638.540	100.134	472.723	811.197	-84.743
600	690.784	957.187	681.870	165.190	467.007	879.459	-76.562
700	756.938	1068.836	729.259	237.703	462.827	948.558	-70.781
800	809.861	1173.492	778.319	316.138	460.007	1018.145	-66.477
900	852.865	1271.447	827.729	399.346	458.373	1088.005	-63.145
1000	888.286	1363.197	876.738	486.459	457.764	1158.005	-60.487
1100	917.784	1449.285	924.916	576.806	457.979	1228.036	-58.313
1200	942.569	1530.236	972.020	669.859	458.878	1297.995	-56.499
1300	963.553	1606.533	1017.922	765.194	460.275	1367.871	-54.961
1400	981.435	1678.612	1062.564	862.466	462.036	1437.629	-53.637
1500	996.766	1746.860	1105.929	961.396	464.081	1507.253	-52.486
1600	1009.984	1811.622	1148.029	1061.749	466.276	1576.725	-51.474
1700	1021.440	1873.204	1188.890	1163.334	468.549	1646.031	-50.575
1800	1031.419	1931.876	1228.550	1265.988	470.821	1715.272	-49.775
1900	1040.152	1987.882	1267.052	1369.576	473.063	1784.330	-49.054
2000	1047.830	2041.434	1304.442	1473.983	475.220	1853.301	-48.402
2100	1054.609	2092.725	1340.767	1579.112	477.211	1922.152	-47.810
2200	1060.620	2141.927	1376.072	1684.880	479.037	1990.914	-47.269
2300	1065.969	2189.194	1410.405	1791.214	480.693	2059.598	-46.774
2400	1070.748	2234.664	1443.808	1898.054	482.105	2128.161	-46.317
2500	1075.032	2278.462	1476.323	2005.347	483.288	2196.793	-45.899
2600	1078.886	2320.702	1507.992	2113.046	484.204	2265.255	-45.509
2700	1082.363	2361.486	1538.852	2221.112	484.857	2333.769	-45.149
2800	1085.511	2400.907	1568.939	2329.508	485.221	2402.284	-44.814
2900	1088.367	2439.049	1598.289	2438.204	485.265	2470.735	-44.502
3000	1090.968	2475.991	1626.933	2547.173	485.038	2539.219	-44.211
3100	1093.341	2511.803	1654.903	2656.390	484.455	2607.630	-43.937
3200	1095.511	2546.550	1682.227	2765.834	483.564	2676.146	-43.683
3300	1097.502	2580.292	1708.932	2875.487	482.344	2744.739	-43.445
3400	1099.331	2613.083	1735.045	2985.329	480.765	2813.277	-43.220
3500	1101.016	2644.974	1760.589	3095.348	478.833	2881.848	-43.008
3600	1102.571	2676.013	1785.588	3205.528	476.573	2950.576	-42.811
3700	1104.009	2706.242	1810.064	3315.858	473.951	3019.388	-42.625
3800	1105.341	2735.702	1834.037	3426.327	470.940	3088.212	-42.450
3900	1106.578	2764.430	1857.527	3536.923	467.582	3157.061	-42.283
4000	1107.727	2792.461	1880.551	3647.639	463.862	3226.155	-42.128
4100	1108.797	2819.827	1903.128	3758.466	459.741	3295.265	-41.981
4200	1109.796	2846.558	1925.273	3869.396	455.249	3364.471	-41.842
4300	1110.728	2872.683	1947.004	3980.423	450.372	3433.689	-41.710
4400	1111.600	2898.229	1968.333	4091.540	445.119	3503.125	-41.587
4500	1112.418	2923.219	1989.276	4202.741	439.506	3572.745	-41.470
4600	1113.184	2947.677	2009.846	4314.022	433.477	3642.507	-41.361
4700	1113.904	2971.625	2030.056	4425.377	427.048	3712.277	-41.256
4800	1114.581	2995.084	2049.917	4536.801	420.268	3782.305	-41.159
4900	1115.218	3018.072	2069.441	4648.291	413.058	3852.329	-41.065
5000	1115.819	3040.609	2088.640	4759.843	405.521	3922.707	-40.979

3.413. Benzo[*st*]naphtho[2,1,8,7-*defg*]pentacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 14258-76-5
Point Group: C_s

Length: 16.59 Å
Width: 11.14 Å
Breadth: 3.890 Å
L/B Ratio: 1.489

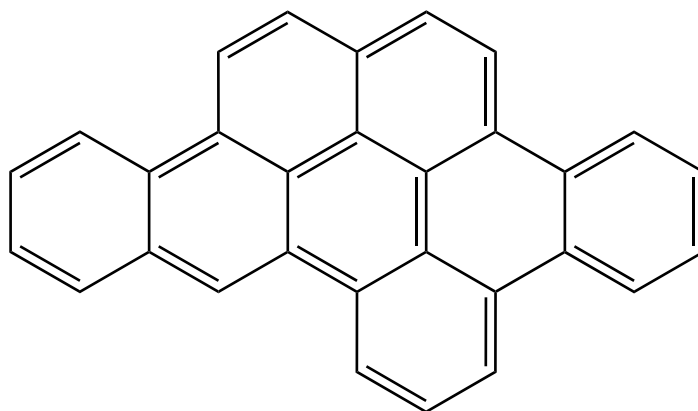
Cartesian coordinates:

C	0.2574	-2.6553	0.0000	C	-4.4758	-0.8392	0.0000	H	1.7384	3.4684	0.0000
C	-0.9864	-3.2422	0.0000	C	-4.5690	-2.2736	0.0000	H	-0.3101	4.8793	0.0000
C	0.4039	-1.2528	0.0000	C	-3.4540	-3.0423	0.0000	H	-2.5635	3.8154	0.0000
C	0.6477	1.6040	0.0000	C	-2.1475	-2.4450	0.0000	H	-4.1860	3.0452	0.0000
C	0.7425	2.9996	0.0000	C	1.8489	0.7763	0.0000	H	-6.4230	1.9596	0.0000
C	-0.3992	3.7880	0.0000	C	1.7280	-0.6444	0.0000	H	-6.6178	-0.5184	0.0000
C	-1.6539	3.1953	0.0000	C	2.8703	-1.4261	0.0000	H	-5.5671	-2.7265	0.0000
C	-0.7383	-0.4440	0.0000	C	3.1072	1.3527	0.0000	H	-3.5222	-4.1362	0.0000
C	-0.6251	0.9974	0.0000	C	4.2744	0.5622	0.0000	H	2.7774	-2.5241	0.0000
C	-1.7838	1.8034	0.0000	C	4.1544	-0.8448	0.0000	H	3.2019	2.4506	0.0000
C	-3.1031	1.1836	0.0000	C	5.3345	-1.6443	0.0000	H	5.2322	-2.7353	0.0000
C	-4.2666	1.9472	0.0000	C	6.5655	-1.0536	0.0000	H	7.4759	-1.6620	0.0000
C	-5.5220	1.3373	0.0000	C	6.6860	0.3599	0.0000	H	7.6862	0.8054	0.0000
C	-5.6316	-0.0404	0.0000	C	5.5727	1.1504	0.0000	H	5.6566	2.2430	0.0000
C	-2.0236	-1.0444	0.0000	H	1.1648	-3.2789	0.0000				
C	-3.2049	-0.2280	0.0000	H	-1.0840	-4.3338	0.0000				

Table 3.413: Table of thermodynamic data as a function of temperature for Benzo[*st*]naphtho[2,1,8,7-*defg*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.966	454.980	454.980	∞
100	115.935	368.659	836.102	-46.744	481.710	528.282	-275.940
200	233.900	483.226	630.936	-29.542	467.580	580.486	-151.604
250	302.139	542.698	607.308	-16.153	460.922	609.482	-127.342
298.15	368.626	601.613	601.613	0.000	454.980	638.649	-111.886
300	371.151	603.901	601.620	0.684	454.761	639.786	-111.394
350	437.576	666.153	606.385	20.919	449.273	671.071	-100.150
400	499.267	728.670	617.764	44.362	444.501	703.080	-91.811
450	555.225	790.765	633.544	70.749	440.360	735.656	-85.391
500	605.287	851.905	652.333	99.786	436.761	768.686	-80.302
600	689.256	969.989	695.521	164.681	430.883	835.653	-72.749
700	755.585	1081.415	742.773	237.050	426.558	903.484	-67.417
800	808.657	1185.901	791.705	315.357	423.611	971.822	-63.452
900	851.784	1283.722	840.999	398.451	421.863	1040.448	-60.385
1000	887.310	1375.363	889.902	485.461	421.152	1109.226	-57.939
1100	916.899	1461.363	937.985	575.716	421.274	1178.045	-55.940
1200	941.764	1542.240	985.003	668.684	422.088	1246.800	-54.271
1300	962.818	1618.476	1030.828	763.942	423.408	1315.479	-52.856
1400	980.763	1690.502	1075.399	861.144	425.098	1384.045	-51.638
1500	996.150	1758.706	1118.700	960.009	427.079	1452.483	-50.579
1600	1009.418	1823.430	1160.740	1060.303	429.216	1520.772	-49.647
1700	1020.919	1884.979	1201.547	1161.834	431.434	1588.899	-48.820
1800	1030.939	1943.623	1241.157	1264.438	433.656	1656.964	-48.083
1900	1039.708	1999.603	1279.613	1367.980	435.852	1724.849	-47.418
2000	1047.419	2053.133	1316.961	1472.344	437.967	1792.648	-46.818
2100	1054.228	2104.405	1353.246	1577.434	439.918	1860.331	-46.272
2200	1060.266	2153.590	1388.515	1683.164	441.707	1927.926	-45.774
2300	1065.640	2200.841	1422.813	1789.465	443.329	1995.444	-45.317
2400	1070.441	2246.298	1456.184	1896.273	444.710	2062.843	-44.896
2500	1074.745	2290.084	1488.670	2003.536	445.863	2130.312	-44.510
2600	1078.617	2332.313	1520.310	2111.208	446.750	2197.613	-44.150
2700	1082.111	2373.087	1551.144	2219.247	447.378	2264.965	-43.817
2800	1085.274	2412.499	1581.207	2327.619	447.717	2332.321	-43.509
2900	1088.145	2450.634	1610.533	2436.292	447.739	2399.613	-43.221
3000	1090.758	2487.568	1639.155	2545.239	447.490	2466.939	-42.952
3100	1093.142	2523.374	1667.104	2654.436	446.886	2534.192	-42.700
3200	1095.324	2558.114	1694.408	2763.861	445.975	2601.552	-42.465
3300	1097.325	2591.850	1721.094	2873.495	444.737	2668.989	-42.246
3400	1099.163	2624.636	1747.189	2983.320	443.141	2736.372	-42.038
3500	1100.857	2656.523	1772.717	3093.323	441.193	2803.787	-41.843
3600	1102.420	2687.558	1797.700	3203.487	438.918	2871.360	-41.661
3700	1103.865	2717.783	1822.160	3313.803	436.281	2939.018	-41.491
3800	1105.204	2747.239	1846.119	3424.257	433.255	3006.688	-41.329
3900	1106.447	2775.963	1869.594	3534.840	429.885	3074.384	-41.176
4000	1107.602	2803.991	1892.605	3645.543	426.152	3142.325	-41.034
4100	1108.678	2831.354	1915.169	3756.358	422.018	3210.282	-40.899
4200	1109.682	2858.082	1937.302	3867.277	417.515	3278.335	-40.771
4300	1110.619	2884.205	1959.021	3978.292	412.627	3346.401	-40.650
4400	1111.496	2909.748	1980.339	4089.398	407.363	3414.685	-40.537
4500	1112.317	2934.735	2001.271	4200.590	401.740	3483.154	-40.431
4600	1113.088	2959.191	2021.831	4311.860	395.701	3551.763	-40.331
4700	1113.812	2983.138	2042.030	4423.206	389.262	3620.382	-40.235
4800	1114.492	3006.594	2061.882	4534.621	382.474	3689.259	-40.146
4900	1115.133	3029.581	2081.397	4646.103	375.255	3758.132	-40.061
5000	1115.737	3052.116	2100.587	4757.646	367.709	3827.360	-39.983

3.414. Benzo[qr]naphtho[2,1,8,7-fghi]pentacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 190-87-4
Point Group: C_s

Length: 16.59 Å
Width: 11.13 Å
Breadth: 3.886 Å
L/B Ratio: 1.490

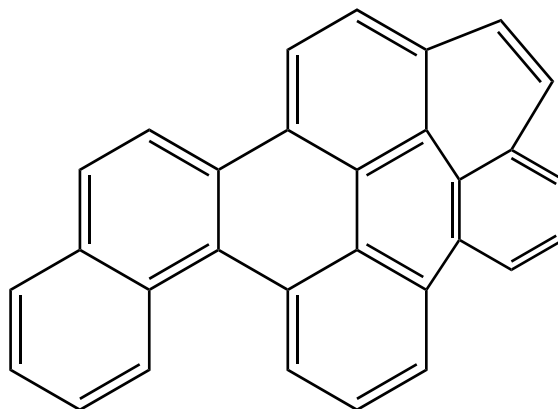
Cartesian coordinates:

C	2.1711	2.7307	0.0000	C	-1.3353	-0.9936	0.0000	H	-0.8743	-3.6421	0.0000
C	0.9574	3.3620	0.0000	C	-2.5019	-1.7157	0.0000	H	1.3390	-4.7785	0.0000
C	-0.0333	-1.6568	0.0000	C	-2.6249	1.0971	0.0000	H	3.4359	-3.4363	0.0000
C	0.0522	-3.0474	0.0000	C	-1.3893	0.4400	0.0000	H	4.9332	-2.4704	0.0000
C	1.2907	-3.6847	0.0000	C	-0.1779	1.2038	0.0000	H	7.0223	-1.1192	0.0000
C	2.4542	-2.9385	0.0000	C	-0.2414	2.6074	0.0000	H	6.8981	1.3657	0.0000
C	1.0909	0.5542	0.0000	C	-1.5131	3.2559	0.0000	H	4.6856	2.5019	0.0000
C	1.1538	-0.8880	0.0000	C	-2.6596	2.5252	0.0000	H	-2.4638	-2.8172	0.0000
C	2.4044	-1.5355	0.0000	C	-3.7705	-1.0718	0.0000	H	-1.5441	4.3515	0.0000
C	2.2610	1.3158	0.0000	C	-3.8420	0.3339	0.0000	H	-3.6461	3.0141	0.0000
C	3.5542	0.6566	0.0000	C	-5.1158	0.9550	0.0000	H	-5.1596	2.0548	0.0000
C	3.6245	-0.7468	0.0000	C	-6.2615	0.2014	0.0000	H	-7.2434	0.6858	0.0000
C	4.8873	-1.3705	0.0000	C	-6.1868	-1.2069	0.0000	H	-7.1120	-1.7923	0.0000
C	6.0463	-0.6232	0.0000	C	-4.9669	-1.8333	0.0000	H	-4.9001	-2.9271	0.0000
C	5.9763	0.7750	0.0000	H	3.1050	3.3136	0.0000				
C	4.7488	1.4031	0.0000	H	0.8974	4.4564	0.0000				

Table 3.414: Table of thermodynamic data as a function of temperature for Benzo[*qr*]naphtho[2,1,8,7-*fghi*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.958	456.048	456.048	∞
100	116.524	365.028	832.619	-46.759	482.763	529.698	-276.680
200	233.957	479.875	627.473	-29.520	468.671	582.247	-152.064
250	301.889	539.326	603.867	-16.135	462.007	611.411	-127.745
298.15	368.173	598.178	598.178	0.000	456.048	640.741	-112.253
300	370.691	600.463	598.185	0.683	455.828	641.885	-111.760
350	436.998	662.634	602.944	20.892	450.314	673.343	-100.489
400	498.634	725.070	614.308	44.305	445.511	705.530	-92.131
450	554.577	787.089	630.067	70.660	441.338	738.288	-85.696
500	604.646	848.161	648.833	99.664	437.707	771.504	-80.597
600	688.653	966.131	691.971	164.496	431.767	838.851	-73.027
700	755.023	1077.468	739.172	236.807	427.384	907.073	-67.685
800	808.131	1181.881	788.056	315.060	424.382	975.809	-63.712
900	851.291	1279.642	837.305	398.103	422.583	1044.840	-60.640
1000	886.847	1371.233	886.167	485.066	421.824	1114.029	-58.190
1100	916.464	1457.189	934.212	575.275	421.901	1183.263	-56.187
1200	941.357	1538.030	981.195	668.201	422.674	1252.438	-54.516
1300	962.438	1614.234	1026.988	763.420	423.954	1321.539	-53.099
1400	980.408	1686.233	1071.529	860.585	425.608	1390.531	-51.880
1500	995.820	1754.413	1114.803	959.416	427.554	1459.396	-50.820
1600	1009.111	1819.117	1156.818	1059.679	429.659	1528.115	-49.887
1700	1020.634	1880.648	1197.601	1161.180	431.848	1596.675	-49.059
1800	1030.673	1939.276	1237.189	1263.756	434.042	1665.174	-48.321
1900	1039.461	1995.242	1275.625	1367.272	436.213	1733.494	-47.656
2000	1047.189	2048.760	1312.954	1471.613	438.303	1801.730	-47.055
2100	1054.013	2100.021	1349.221	1576.680	440.232	1869.851	-46.509
2200	1060.064	2149.197	1384.474	1682.390	442.000	1937.885	-46.010
2300	1065.451	2196.439	1418.756	1788.671	443.603	2005.843	-45.553
2400	1070.264	2241.888	1452.113	1895.461	444.965	2073.682	-45.132
2500	1074.579	2285.668	1484.585	2002.707	446.101	2141.592	-44.745
2600	1078.461	2327.890	1516.212	2110.362	446.973	2209.335	-44.385
2700	1081.965	2368.659	1547.034	2218.387	447.585	2277.130	-44.053
2800	1085.136	2408.065	1577.085	2326.744	447.911	2344.929	-43.744
2900	1088.015	2446.195	1606.401	2435.404	447.918	2412.665	-43.456
3000	1090.635	2483.125	1635.013	2544.339	447.657	2480.435	-43.187
3100	1093.026	2518.927	1662.951	2653.524	447.042	2548.133	-42.935
3200	1095.214	2553.664	1690.246	2762.937	446.120	2615.937	-42.700
3300	1097.221	2587.397	1716.924	2872.560	444.871	2683.819	-42.480
3400	1099.065	2620.180	1743.010	2982.376	443.264	2751.647	-42.273
3500	1100.763	2652.064	1768.530	3092.368	441.307	2819.508	-42.078
3600	1102.331	2683.096	1793.505	3202.524	439.022	2887.528	-41.896
3700	1103.780	2713.318	1817.959	3312.831	436.377	2955.632	-41.725
3800	1105.123	2742.772	1841.910	3423.277	433.343	3023.749	-41.563
3900	1106.370	2771.495	1865.379	3533.852	429.964	3091.891	-41.410
4000	1107.529	2799.520	1888.383	3644.548	426.224	3160.279	-41.268
4100	1108.608	2826.881	1910.941	3755.355	422.083	3228.683	-41.133
4200	1109.614	2853.608	1933.069	3866.267	417.573	3297.184	-41.006
4300	1110.555	2879.729	1954.781	3977.276	412.678	3365.697	-40.884
4400	1111.434	2905.271	1976.094	4088.376	407.408	3434.429	-40.771
4500	1112.258	2930.257	1997.021	4199.561	401.779	3503.345	-40.665
4600	1113.031	2954.712	2017.576	4310.826	395.734	3572.403	-40.565
4700	1113.757	2978.657	2037.771	4422.165	389.290	3641.470	-40.470
4800	1114.440	3002.112	2057.617	4533.576	382.496	3710.795	-40.381
4900	1115.082	3025.098	2077.128	4645.052	375.272	3780.116	-40.296
5000	1115.688	3047.632	2096.314	4756.591	367.721	3849.792	-40.218

3.415. Benzo[*pqr*]naphtho[2,1-*b*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-56-5
Point Group: C₁

Length: 15.90 Å
Width: 10.42 Å
Breadth: 5.033 Å
L/B Ratio: 1.526

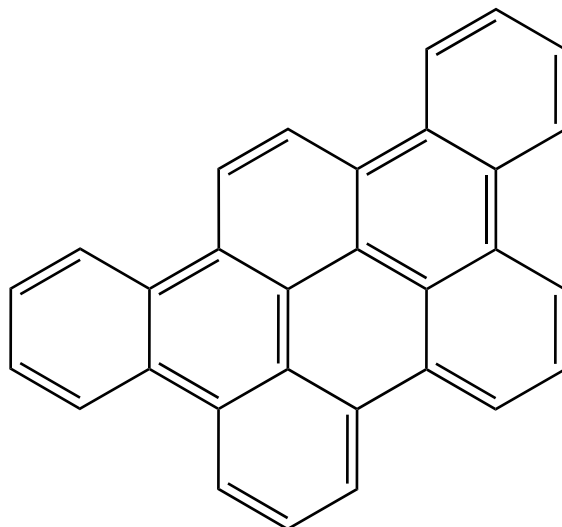
Cartesian coordinates:

C	4.0058	1.3919	0.5947	C	-0.8306	3.1079	-0.3958	H	0.8377	4.4041	-0.8238
C	3.4624	0.1722	0.1126	C	-1.2543	1.7988	-0.1838	H	-1.9657	-4.3230	-0.0080
C	4.3616	-0.9011	-0.0675	C	-2.1317	-0.9087	0.0334	H	0.4442	-3.8128	-0.2560
C	5.7559	-0.7110	0.1030	C	-3.0909	0.1556	0.0964	H	-3.2995	3.5627	-0.0339
C	6.2473	0.5000	0.5148	C	-2.6719	1.5035	-0.0087	H	-5.7089	3.0264	0.2701
C	5.3539	1.5533	0.7892	C	-2.5687	-2.2408	0.0796	H	-6.4604	0.6635	0.4377
C	3.8658	-2.2020	-0.3706	C	-1.6213	-3.2828	-0.0300	H	-5.9413	-1.7325	0.4444
C	2.5265	-2.4246	-0.3935	C	-0.2868	-2.9954	-0.1638	H	-4.2813	-3.5730	0.2781
C	1.5965	-1.3539	-0.2333	C	-4.4596	-0.1463	0.2475	H	2.1338	-3.4402	-0.5528
C	2.0513	-0.0390	-0.1201	C	-5.3975	0.8995	0.3136	H	4.5780	-3.0169	-0.5437
C	0.1806	-1.6591	-0.1771	C	-4.9786	2.2120	0.2189	H	6.4318	-1.5527	-0.0873
C	-0.7454	-0.6153	-0.0841	C	-3.6247	2.5145	0.0532	H	7.3226	0.6536	0.6495
C	-0.3010	0.7512	-0.1551	C	-3.9671	-2.5239	0.2326	H	5.7467	2.5036	1.1659
C	1.0804	1.0403	-0.2458	C	-4.8732	-1.5195	0.3211	H	3.3321	2.2262	0.8329
C	1.4532	2.3646	-0.5319	H	-1.5749	3.9187	-0.4132				
C	0.5173	3.3801	-0.6043	H	2.5094	2.6101	-0.7080				

Table 3.415: Table of thermodynamic data as a function of temperature for Benzo[*pqr*]naphtho[2,1-*b*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.533	477.110	477.110	∞
100	114.019	356.864	823.071	-46.621	503.963	551.715	-288.180
200	233.426	470.613	618.253	-29.528	489.724	605.153	-158.046
250	302.021	530.020	594.631	-16.153	483.051	634.781	-132.628
298.15	368.737	588.936	588.936	0.000	477.110	664.558	-116.425
300	371.269	591.224	588.943	0.685	476.891	665.719	-115.910
350	437.858	653.507	593.709	20.929	471.413	697.637	-104.114
400	499.658	716.070	605.095	44.390	466.658	730.277	-95.362
450	555.683	778.214	620.885	70.798	462.538	763.482	-88.621
500	605.779	839.405	639.687	99.859	458.963	797.138	-83.275
600	689.751	957.580	682.908	164.803	453.135	865.351	-75.334
700	756.035	1069.080	730.194	237.220	448.858	934.419	-69.726
800	809.046	1173.621	779.160	315.569	445.953	1003.987	-65.552
900	852.112	1271.484	828.486	398.699	444.241	1073.839	-62.323
1000	887.584	1363.158	877.419	485.739	443.559	1143.839	-59.747
1100	917.126	1449.181	925.528	576.018	443.706	1213.877	-57.641
1200	941.953	1530.076	972.570	669.007	444.542	1283.850	-55.883
1300	962.975	1606.326	1018.416	764.282	445.878	1353.744	-54.393
1400	980.895	1678.363	1063.006	861.499	447.583	1423.525	-53.111
1500	996.261	1746.575	1106.324	960.376	449.576	1493.176	-51.996
1600	1009.513	1811.305	1148.380	1060.681	451.723	1562.678	-51.015
1700	1021.000	1872.860	1189.201	1162.220	453.950	1632.017	-50.145
1800	1031.009	1931.508	1228.824	1264.832	456.180	1701.294	-49.369
1900	1039.769	1987.492	1267.292	1368.380	458.382	1770.390	-48.670
2000	1047.472	2041.025	1304.650	1472.751	460.503	1839.401	-48.039
2100	1054.275	2092.299	1340.945	1577.845	462.459	1908.294	-47.465
2200	1060.307	2141.486	1376.223	1683.580	464.252	1977.099	-46.941
2300	1065.676	2188.739	1410.529	1789.884	465.878	2045.828	-46.461
2400	1070.473	2234.197	1443.907	1896.696	467.262	2114.436	-46.019
2500	1074.774	2277.985	1476.400	2003.962	468.418	2183.116	-45.613
2600	1078.643	2320.215	1508.047	2111.636	469.308	2251.626	-45.235
2700	1082.135	2360.990	1538.887	2219.678	469.938	2320.189	-44.886
2800	1085.295	2400.403	1568.955	2328.052	470.280	2388.754	-44.562
2900	1088.164	2438.538	1598.287	2436.728	470.304	2457.256	-44.259
3000	1090.776	2475.473	1626.914	2545.677	470.057	2525.791	-43.977
3100	1093.159	2511.279	1654.868	2654.875	469.455	2594.254	-43.712
3200	1095.339	2546.020	1682.176	2764.302	468.546	2662.823	-43.465
3300	1097.339	2579.757	1708.867	2873.937	467.309	2731.469	-43.235
3400	1099.176	2612.543	1734.966	2983.764	465.714	2800.061	-43.017
3500	1100.869	2644.430	1760.497	3093.768	463.768	2868.686	-42.812
3600	1102.431	2675.465	1785.484	3203.934	461.494	2937.469	-42.621
3700	1103.876	2705.691	1809.947	3314.250	458.858	3006.336	-42.441
3800	1105.214	2735.147	1833.909	3424.705	455.833	3075.215	-42.271
3900	1106.456	2763.872	1857.387	3535.289	452.464	3144.120	-42.110
4000	1107.611	2791.899	1880.401	3645.994	448.732	3213.270	-41.960
4100	1108.687	2819.263	1902.968	3756.809	444.599	3282.436	-41.818
4200	1109.690	2845.991	1925.104	3867.728	440.096	3351.698	-41.684
4300	1110.627	2872.114	1946.825	3978.745	435.209	3420.974	-41.556
4400	1111.503	2897.657	1968.145	4089.852	429.946	3490.467	-41.436
4500	1112.324	2922.645	1989.080	4201.044	424.324	3560.144	-41.324
4600	1113.094	2947.101	2009.641	4312.315	418.285	3629.963	-41.219
4700	1113.818	2971.047	2029.843	4423.661	411.847	3699.791	-41.118
4800	1114.498	2994.504	2049.697	4535.077	405.059	3769.877	-41.024
4900	1115.138	3017.491	2069.214	4646.559	397.841	3839.958	-40.934
5000	1115.742	3040.026	2088.405	4758.103	390.295	3910.395	-40.851

3.416. Tribenzo[*b,n,pqr*]perylene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 190-81-8
Point Group: C_{2v}

Length: 15.92 Å
Width: 10.42 Å
Breadth: 3.885 Å
L/B Ratio: 1.528

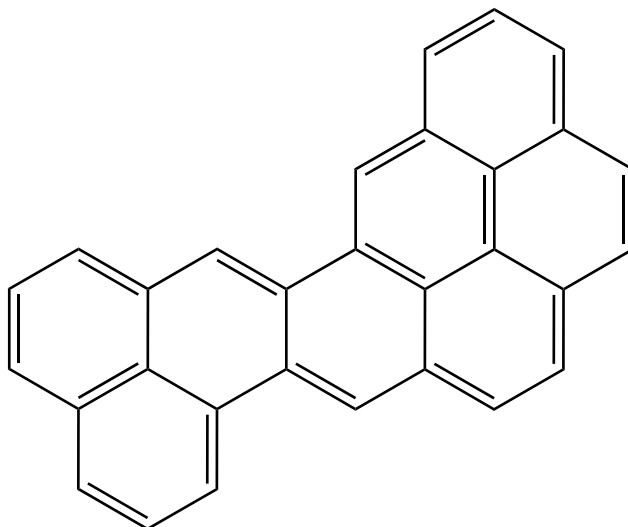
Cartesian coordinates:

C	0.6994	-2.6724	0.0000	C	-2.8449	0.9919	0.0000	H	4.6169	2.2396	0.0000
C	-0.6771	-2.6781	0.0000	C	-1.4032	-1.4744	0.0000	H	3.3597	4.3873	0.0000
C	1.4154	-1.4627	0.0000	C	-2.8567	-1.4838	0.0000	H	0.8725	4.3813	0.0000
C	2.8366	1.0156	0.0000	C	-3.5657	-0.2713	0.0000	H	-0.9090	4.3739	0.0000
C	3.5162	2.2396	0.0000	C	-4.9725	-0.2994	0.0000	H	-3.3962	4.3592	0.0000
C	2.8173	3.4362	0.0000	C	-5.6574	-1.4978	0.0000	H	-4.6354	2.2010	0.0000
C	1.4284	3.4313	0.0000	C	-4.9513	-2.7052	0.0000	H	-5.5208	0.6551	0.0000
C	0.7101	-0.2483	0.0000	C	-3.5712	-2.6962	0.0000	H	-6.7521	-1.5068	0.0000
C	1.4258	1.0052	0.0000	C	3.5679	-0.2416	0.0000	H	-5.4961	-3.6548	0.0000
C	0.7193	2.2277	0.0000	C	2.8689	-1.4599	0.0000	H	-3.0085	-3.6422	0.0000
C	-0.7378	2.2217	0.0000	C	3.5935	-2.6663	0.0000	H	3.0387	-3.6170	0.0000
C	-1.4569	3.4192	0.0000	C	4.9737	-2.6638	0.0000	H	5.5263	-3.6089	0.0000
C	-2.8458	3.4126	0.0000	C	5.6696	-1.4506	0.0000	H	6.7644	-1.4505	0.0000
C	-3.5347	2.2103	0.0000	C	4.9748	-0.2580	0.0000	H	5.5151	0.7011	0.0000
C	-0.7080	-0.2542	0.0000	H	1.2589	-3.6205	0.0000				
C	-1.4341	0.9933	0.0000	H	-1.2286	-3.6309	0.0000				

Table 3.416: Table of thermodynamic data as a function of temperature for Tribenzo[*b,n,pqr*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-54.051	455.480	455.480	∞
100	117.120	361.082	828.881	-46.780	482.174	529.504	-276.579
200	234.022	476.187	623.717	-29.506	468.116	582.430	-152.112
250	301.729	535.625	600.124	-16.125	461.450	611.778	-127.821
298.15	367.915	594.439	594.439	0.000	455.480	641.288	-112.349
300	370.432	596.723	594.446	0.683	455.259	642.439	-111.856
350	436.736	658.853	599.202	20.878	449.732	674.085	-100.600
400	498.414	721.256	610.559	44.279	444.917	706.462	-92.253
450	554.412	783.252	626.310	70.624	440.734	739.411	-85.827
500	604.530	844.310	645.066	99.622	437.096	772.819	-80.734
600	688.599	962.265	688.189	164.446	431.148	840.553	-73.175
700	754.988	1073.595	735.377	236.753	426.761	909.161	-67.841
800	808.092	1178.003	784.251	315.002	423.756	978.284	-63.874
900	851.238	1275.759	833.492	398.040	421.953	1047.704	-60.806
1000	886.780	1367.344	882.347	484.997	421.187	1117.281	-58.360
1100	916.385	1453.293	930.385	575.199	421.257	1186.904	-56.360
1200	941.269	1534.127	977.363	668.117	422.021	1256.469	-54.692
1300	962.344	1610.323	1023.150	763.326	423.292	1325.961	-53.277
1400	980.312	1682.316	1067.686	860.482	424.936	1395.344	-52.060
1500	995.723	1750.489	1110.954	959.303	426.873	1464.602	-51.001
1600	1009.015	1815.186	1152.964	1059.556	428.968	1533.714	-50.070
1700	1020.540	1876.711	1193.742	1161.047	431.148	1602.666	-49.243
1800	1030.582	1935.334	1233.326	1263.615	433.333	1671.559	-48.506
1900	1039.373	1991.296	1271.758	1367.122	435.494	1740.274	-47.842
2000	1047.105	2044.809	1309.082	1471.454	437.576	1808.905	-47.243
2100	1053.933	2096.066	1345.346	1576.513	439.497	1877.421	-46.697
2200	1059.988	2145.238	1380.595	1682.215	441.257	1945.850	-46.199
2300	1065.378	2192.477	1414.874	1788.488	442.853	2014.205	-45.743
2400	1070.195	2237.923	1448.227	1895.271	444.208	2082.440	-45.322
2500	1074.514	2281.700	1480.696	2002.511	445.337	2150.747	-44.936
2600	1078.399	2323.920	1512.320	2110.160	446.202	2218.887	-44.577
2700	1081.905	2364.686	1543.139	2218.178	446.808	2287.079	-44.245
2800	1085.080	2404.091	1573.187	2326.530	447.128	2355.276	-43.937
2900	1087.961	2442.219	1602.500	2435.184	447.130	2423.409	-43.649
3000	1090.584	2479.147	1631.109	2544.113	446.864	2491.576	-43.381
3100	1092.978	2514.947	1659.046	2653.293	446.243	2559.672	-43.129
3200	1095.168	2549.683	1686.338	2762.702	445.316	2627.875	-42.895
3300	1097.176	2583.414	1713.014	2872.321	444.063	2696.155	-42.676
3400	1099.022	2616.196	1739.098	2982.132	442.452	2764.382	-42.469
3500	1100.723	2648.078	1764.615	3092.120	440.491	2832.641	-42.274
3600	1102.292	2679.109	1789.589	3202.272	438.202	2901.059	-42.092
3700	1103.743	2709.331	1814.040	3312.575	435.553	2969.562	-41.922
3800	1105.088	2738.784	1837.990	3423.017	432.516	3038.078	-41.760
3900	1106.336	2767.505	1861.457	3533.589	429.134	3106.619	-41.608
4000	1107.496	2795.530	1884.460	3644.282	425.390	3175.406	-41.466
4100	1108.577	2822.891	1907.016	3755.086	421.246	3244.209	-41.331
4200	1109.585	2849.617	1929.142	3865.995	416.733	3313.109	-41.204
4300	1110.526	2875.737	1950.853	3977.001	411.835	3382.021	-41.083
4400	1111.407	2901.278	1972.165	4088.098	406.562	3451.152	-40.970
4500	1112.232	2926.263	1993.090	4199.280	400.930	3520.468	-40.864
4600	1113.006	2950.718	2013.643	4310.542	394.883	3589.925	-40.764
4700	1113.733	2974.662	2033.837	4421.880	388.436	3659.391	-40.669
4800	1114.416	2998.117	2053.682	4533.288	381.640	3729.116	-40.580
4900	1115.060	3021.102	2073.192	4644.762	374.414	3798.836	-40.495
5000	1115.666	3043.636	2092.376	4756.298	366.861	3868.912	-40.417

3.417. Benzo[*kl*]naphtho[2,1,8,7-*defg*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-70-3
Point Group: C_s

Length: 15.97 Å
Width: 10.39 Å
Breadth: 3.885 Å
L/B Ratio: 1.537

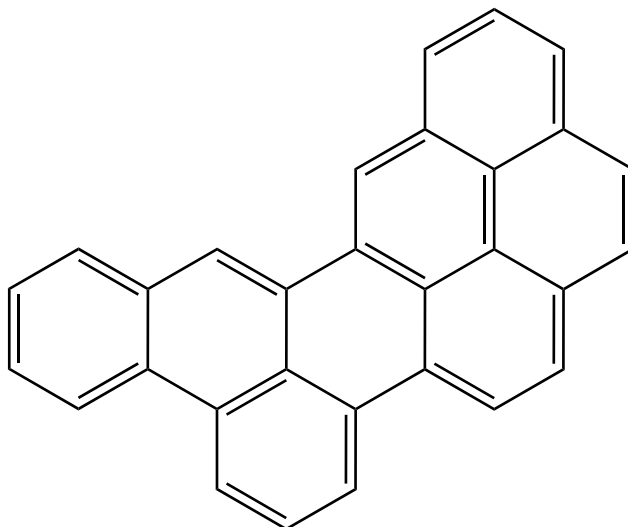
Cartesian coordinates:

C	-3.3365	-2.9891	0.0000	C	-0.6877	1.9925	0.0000	H	-5.2390	-3.9966	0.0000
C	-5.4728	-1.8569	0.0000	C	1.5078	0.9102	0.0000	H	-0.6560	-2.6224	0.0000
C	-4.7263	-3.0287	0.0000	C	0.8829	-0.4100	0.0000	H	-0.9301	4.1414	0.0000
C	-2.6674	-1.7609	0.0000	C	1.6380	-1.5370	0.0000	H	-3.4088	4.0560	0.0000
C	-1.2335	-1.6836	0.0000	C	3.0822	-1.4942	0.0000	H	-5.5000	2.7563	0.0000
C	-1.4449	3.1737	0.0000	C	3.8350	-2.6522	0.0000	H	-6.6657	0.5662	0.0000
C	-2.8274	3.1269	0.0000	C	5.2418	-2.5858	0.0000	H	1.2439	3.0265	0.0000
C	-3.4199	-0.5642	0.0000	C	5.8847	-1.3741	0.0000	H	1.1494	-2.5255	0.0000
C	-2.7477	0.6992	0.0000	C	3.7298	-0.2251	0.0000	H	3.3425	-3.6312	0.0000
C	-3.4975	1.8947	0.0000	C	5.1391	-0.1670	0.0000	H	5.8179	-3.5171	0.0000
C	-4.9346	1.8172	0.0000	C	5.7842	1.0988	0.0000	H	6.9793	-1.3212	0.0000
C	-5.5711	0.6222	0.0000	C	5.0411	2.2489	0.0000	H	6.8793	1.1364	0.0000
C	-4.8317	-0.6135	0.0000	C	3.6322	2.1929	0.0000	H	5.5323	3.2276	0.0000
C	-1.3346	0.7470	0.0000	C	2.9697	0.9821	0.0000	H	3.0496	3.1271	0.0000
C	-0.5792	-0.4850	0.0000	H	-2.7605	-3.9213	0.0000				
C	0.7541	2.0387	0.0000	H	-6.5677	-1.9023	0.0000				

Table 3.417: Table of thermodynamic data as a function of temperature for Benzo[*kl*]naphtho[2,1,8,7-*defg*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.720	511.277	511.277	∞
100	114.436	362.972	830.316	-46.734	538.017	585.157	-305.648
200	234.012	477.012	625.006	-29.599	523.820	637.969	-166.617
250	302.768	536.570	601.329	-16.190	517.182	667.274	-139.416
298.15	369.503	595.620	595.620	0.000	511.277	696.732	-122.062
300	372.034	597.914	595.627	0.686	511.059	697.881	-121.509
350	438.544	660.309	600.403	20.967	505.618	729.461	-108.864
400	500.228	722.956	611.808	44.459	500.894	761.759	-99.474
450	556.141	785.161	627.620	70.893	496.801	794.618	-92.235
500	606.146	846.395	646.446	99.975	493.246	827.926	-86.491
600	690.011	964.626	689.710	164.949	487.449	895.437	-77.953
700	756.264	1076.163	737.034	237.390	483.195	963.798	-71.918
800	809.283	1180.736	786.033	315.762	480.314	1032.656	-67.424
900	852.371	1278.628	835.387	398.917	478.626	1101.795	-63.945
1000	887.863	1370.329	884.345	485.984	477.971	1171.080	-61.170
1100	917.420	1456.380	932.478	576.292	478.147	1240.399	-58.900
1200	942.254	1537.301	979.542	669.311	479.012	1309.651	-57.006
1300	963.278	1613.575	1025.408	764.616	480.379	1378.822	-55.401
1400	981.194	1685.634	1070.018	861.863	482.114	1447.876	-54.020
1500	996.553	1753.867	1113.353	960.770	484.137	1516.799	-52.819
1600	1009.795	1818.616	1155.426	1061.103	486.313	1585.570	-51.762
1700	1021.271	1880.187	1196.263	1162.670	488.567	1654.178	-50.826
1800	1031.267	1938.850	1235.901	1265.308	490.823	1722.721	-49.991
1900	1040.015	1994.848	1274.384	1368.882	493.051	1791.082	-49.239
2000	1047.706	2048.393	1311.755	1473.276	495.195	1859.357	-48.560
2100	1054.496	2099.679	1348.063	1578.393	497.174	1927.513	-47.943
2200	1060.516	2148.875	1383.353	1684.149	498.989	1995.580	-47.380
2300	1065.874	2196.138	1417.671	1790.474	500.635	2063.569	-46.864
2400	1070.660	2241.604	1451.060	1897.305	502.039	2131.437	-46.389
2500	1074.951	2285.399	1483.563	2004.590	503.213	2199.376	-45.952
2600	1078.811	2327.636	1515.220	2112.281	504.120	2267.145	-45.547
2700	1082.294	2368.417	1546.069	2220.339	504.767	2334.965	-45.172
2800	1085.446	2407.835	1576.146	2328.729	505.124	2402.787	-44.824
2900	1088.307	2445.976	1605.486	2437.419	505.162	2470.545	-44.498
3000	1090.911	2482.916	1634.122	2546.382	504.929	2538.336	-44.195
3100	1093.288	2518.726	1662.083	2655.594	504.341	2606.055	-43.911
3200	1095.462	2553.471	1689.398	2765.033	503.444	2673.879	-43.646
3300	1097.455	2587.211	1716.096	2874.680	502.219	2741.780	-43.398
3400	1099.287	2620.001	1742.202	2984.518	500.636	2809.626	-43.164
3500	1100.975	2651.891	1767.739	3094.532	498.700	2877.505	-42.944
3600	1102.532	2682.929	1792.732	3204.709	496.436	2945.542	-42.738
3700	1103.972	2713.157	1817.202	3315.035	493.810	3013.662	-42.544
3800	1105.306	2742.616	1841.169	3425.500	490.795	3081.795	-42.361
3900	1106.544	2771.343	1864.653	3536.093	487.434	3149.953	-42.188
4000	1107.695	2799.373	1887.672	3646.806	483.711	3218.355	-42.027
4100	1108.767	2826.738	1910.243	3757.629	479.587	3286.774	-41.873
4200	1109.767	2853.469	1932.384	3868.557	475.092	3355.289	-41.728
4300	1110.700	2879.593	1954.109	3979.580	470.212	3423.816	-41.590
4400	1111.574	2905.138	1975.435	4090.695	464.956	3492.561	-41.461
4500	1112.392	2930.127	1996.373	4201.893	459.341	3561.490	-41.340
4600	1113.160	2954.585	2016.939	4313.171	453.309	3630.561	-41.225
4700	1113.881	2978.533	2037.145	4424.524	446.877	3699.640	-41.116
4800	1114.558	3001.991	2057.002	4535.946	440.095	3768.978	-41.014
4900	1115.197	3024.979	2076.523	4647.434	432.883	3838.311	-40.916
5000	1115.798	3047.515	2095.718	4758.984	425.343	3907.999	-40.826

3.418. Benzo[*ij*]naphtho[2,1,8,7-*defg*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 105786-27-4
Point Group: C_s

Length: 15.93 Å
Width: 10.41 Å
Breadth: 3.890 Å
L/B Ratio: 1.530

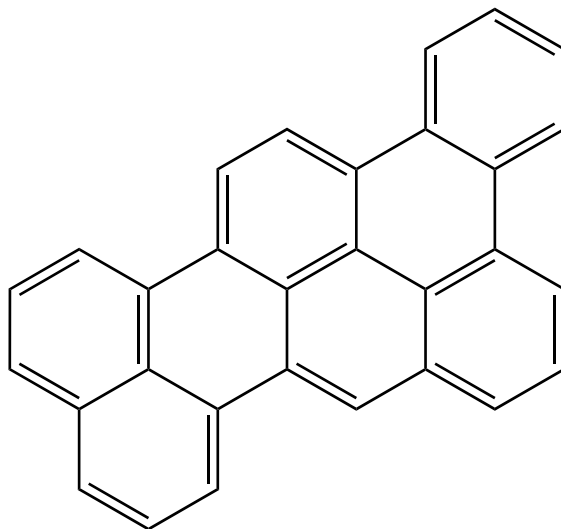
Cartesian coordinates:

C	1.1125	-0.4953	0.0000	C	-4.4496	-3.1975	0.0000	H	3.4748	4.2966	0.0000
C	1.8813	-1.6243	0.0000	C	-3.0615	-3.1333	0.0000	H	0.9943	4.1438	0.0000
C	1.7413	0.8033	0.0000	C	-3.1843	-0.7084	0.0000	H	-0.3926	-2.7214	0.0000
C	3.1471	0.8967	0.0000	C	-2.5307	0.5660	0.0000	H	-0.7839	4.0398	0.0000
C	3.7589	2.1664	0.0000	C	-3.3082	1.7448	0.0000	H	-3.2623	3.9075	0.0000
C	2.9952	3.3123	0.0000	C	-4.7445	1.6421	0.0000	H	-6.3093	-2.1014	0.0000
C	1.5998	3.2244	0.0000	C	-5.3593	0.4369	0.0000	H	-4.9461	-4.1737	0.0000
C	0.9644	1.9901	0.0000	C	-4.5954	-0.7841	0.0000	H	-2.4685	-4.0548	0.0000
C	-0.3483	-0.5827	0.0000	C	3.9494	-0.3069	0.0000	H	-5.3253	2.5717	0.0000
C	-0.9830	-1.7906	0.0000	C	3.3102	-1.5581	0.0000	H	-6.4526	0.3598	0.0000
C	-1.1174	0.6420	0.0000	C	4.0844	-2.7398	0.0000	H	3.5771	-3.7112	0.0000
C	-0.4943	1.9004	0.0000	C	5.4583	-2.6686	0.0000	H	6.0599	-3.5834	0.0000
C	-1.2835	3.0586	0.0000	C	6.1006	-1.4188	0.0000	H	7.1946	-1.3750	0.0000
C	-2.6655	2.9883	0.0000	C	5.3602	-0.2592	0.0000	H	5.8518	0.7257	0.0000
C	-2.4145	-1.8929	0.0000	H	1.4003	-2.6161	0.0000				
C	-5.2153	-2.0376	0.0000	H	4.8585	2.2208	0.0000				

Table 3.418: Table of thermodynamic data as a function of temperature for Benzo[*ij*]naphtho[2,1,8,7-*defg*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.817	472.731	472.731	∞
100	115.507	366.608	833.606	-46.700	499.505	546.282	-285.343
200	233.708	480.984	628.603	-29.524	485.349	598.704	-156.362
250	301.959	540.415	604.989	-16.144	478.682	627.813	-131.172
298.15	368.430	599.297	599.297	0.000	472.731	657.090	-115.117
300	370.954	601.584	599.304	0.684	472.511	658.232	-114.606
350	437.357	663.804	604.067	20.908	467.013	689.633	-102.920
400	499.031	726.291	615.440	44.340	462.229	721.760	-94.250
450	554.981	788.356	631.212	70.715	458.076	754.456	-87.573
500	605.044	849.471	649.992	99.740	454.465	787.607	-82.279
600	689.034	967.512	693.161	164.611	448.564	854.820	-74.417
700	755.393	1078.907	740.393	236.959	444.219	922.900	-68.866
800	808.497	1183.369	789.308	315.249	441.254	991.490	-64.736
900	851.653	1281.173	838.586	398.328	439.491	1060.370	-61.541
1000	887.203	1372.802	887.475	485.327	438.768	1129.404	-58.993
1100	916.812	1458.792	935.545	575.571	438.881	1198.479	-56.910
1200	941.693	1539.662	982.552	668.532	439.687	1267.492	-55.171
1300	962.759	1615.893	1028.367	763.783	441.000	1336.429	-53.697
1400	980.714	1687.915	1072.929	860.980	442.685	1405.254	-52.430
1500	996.110	1756.116	1116.222	959.841	444.662	1473.950	-51.326
1600	1009.384	1820.837	1158.255	1060.131	446.795	1542.498	-50.356
1700	1020.891	1882.384	1199.056	1161.659	449.010	1610.885	-49.495
1800	1030.914	1941.027	1238.660	1264.260	451.229	1679.209	-48.728
1900	1039.688	1997.006	1277.111	1367.800	453.423	1747.354	-48.037
2000	1047.402	2050.535	1314.454	1472.163	455.536	1815.413	-47.413
2100	1054.213	2101.806	1350.735	1577.250	457.485	1883.355	-46.845
2200	1060.252	2150.990	1386.000	1682.979	459.273	1951.210	-46.327
2300	1065.628	2198.241	1420.294	1789.279	460.894	2018.989	-45.852
2400	1070.430	2243.697	1453.662	1896.086	462.273	2086.647	-45.414
2500	1074.736	2287.483	1486.144	2003.348	463.425	2154.377	-45.012
2600	1078.609	2329.712	1517.782	2111.019	464.312	2221.938	-44.638
2700	1082.104	2370.486	1548.613	2219.057	464.938	2289.550	-44.293
2800	1085.267	2409.897	1578.673	2327.428	465.277	2357.166	-43.973
2900	1088.138	2448.032	1607.997	2436.101	465.298	2424.718	-43.673
3000	1090.752	2484.966	1636.617	2545.047	465.049	2492.304	-43.394
3100	1093.137	2520.771	1664.564	2654.244	464.445	2559.818	-43.132
3200	1095.319	2555.512	1691.866	2763.668	463.533	2627.438	-42.888
3300	1097.320	2589.248	1718.550	2873.301	462.295	2695.135	-42.660
3400	1099.159	2622.034	1744.643	2983.127	460.698	2762.778	-42.444
3500	1100.853	2653.920	1770.169	3093.129	458.750	2830.454	-42.241
3600	1102.416	2684.955	1795.151	3203.293	456.474	2898.288	-42.052
3700	1103.862	2715.180	1819.610	3313.608	453.837	2966.205	-41.874
3800	1105.201	2744.636	1843.567	3424.062	450.811	3034.136	-41.706
3900	1106.444	2773.360	1867.041	3534.645	447.440	3102.092	-41.547
4000	1107.600	2801.388	1890.051	3645.348	443.707	3170.293	-41.399
4100	1108.676	2828.750	1912.613	3756.162	439.573	3238.510	-41.258
4200	1109.680	2855.479	1934.746	3867.081	435.070	3306.824	-41.126
4300	1110.617	2881.601	1956.463	3978.096	430.181	3375.150	-40.999
4400	1111.494	2907.144	1977.780	4089.202	424.917	3443.695	-40.881
4500	1112.316	2932.132	1998.711	4200.393	419.294	3512.424	-40.770
4600	1113.086	2956.588	2019.270	4311.663	413.255	3581.294	-40.666
4700	1113.810	2980.534	2039.468	4423.009	406.816	3650.173	-40.566
4800	1114.491	3003.991	2059.319	4534.424	400.027	3719.310	-40.474
4900	1115.131	3026.977	2078.833	4645.905	392.809	3788.443	-40.384
5000	1115.735	3049.512	2098.022	4757.449	385.262	3857.931	-40.303

3.419. Tribenzo[*de,ij,rst*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-65-6
Point Group: C_s

Length: 15.95 Å
Width: 10.41 Å
Breadth: 3.889 Å
L/B Ratio: 1.532

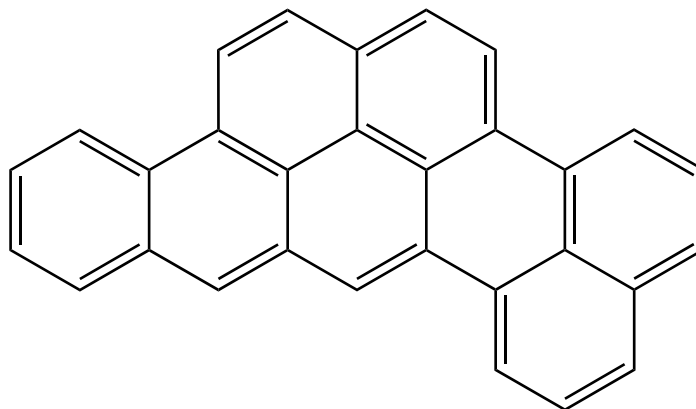
Cartesian coordinates:

C	2.6389	-1.3865	0.0000	C	-0.9113	2.3364	0.0000	H	6.5469	-1.4120	0.0000
C	3.3397	-2.5754	0.0000	C	-1.5988	3.5612	0.0000	H	6.5773	1.0298	0.0000
C	4.7482	-2.5870	0.0000	C	-2.9815	3.5794	0.0000	H	5.3549	3.1973	0.0000
C	5.4510	-1.4115	0.0000	C	-3.7026	2.3859	0.0000	H	2.8720	3.2376	0.0000
C	3.3527	-0.1517	0.0000	C	-0.9242	-0.1242	0.0000	H	-1.4952	-3.4941	0.0000
C	4.7640	-0.1691	0.0000	C	-1.6336	1.1256	0.0000	H	0.9950	-3.5126	0.0000
C	5.4818	1.0566	0.0000	C	-3.0481	1.1561	0.0000	H	1.0718	3.2547	0.0000
C	4.8084	2.2484	0.0000	C	-1.6421	-1.3425	0.0000	H	-1.0321	4.4991	0.0000
C	3.3992	2.2711	0.0000	C	-3.0980	-1.3220	0.0000	H	-3.5178	4.5341	0.0000
C	2.6689	1.1003	0.0000	C	-3.7880	-0.0978	0.0000	H	-4.8033	2.4050	0.0000
C	1.1779	-1.3648	0.0000	C	-5.1932	-0.1010	0.0000	H	-5.7228	0.8642	0.0000
C	-0.9366	-2.5454	0.0000	C	-5.8988	-1.2890	0.0000	H	-6.9936	-1.2787	0.0000
C	0.4512	-2.5551	0.0000	C	-5.2135	-2.5066	0.0000	H	-5.7731	-3.4476	0.0000
C	0.4891	-0.1341	0.0000	C	-3.8319	-2.5209	0.0000	H	-3.2841	-3.4758	0.0000
C	1.2063	1.1205	0.0000	H	2.7890	-3.5287	0.0000				
C	0.5209	2.2999	0.0000	H	5.2719	-3.5487	0.0000				

Table 3.419: Table of thermodynamic data as a function of temperature for Tribenzo[*de,ij,rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.947	476.672	476.672	∞
100	116.289	364.427	832.349	-46.792	503.354	550.349	-287.467
200	234.141	479.252	627.020	-29.554	489.261	602.962	-157.474
250	302.242	538.762	603.385	-16.156	482.611	632.155	-132.079
298.15	368.665	597.689	597.689	0.000	476.672	661.511	-115.892
300	371.189	599.977	597.696	0.684	476.453	662.656	-115.376
350	437.606	662.233	602.461	20.920	470.967	694.136	-103.592
400	499.315	724.756	613.841	44.366	466.196	726.341	-94.848
450	555.298	786.857	629.622	70.756	462.058	759.113	-88.114
500	605.380	848.007	648.413	99.797	458.463	792.338	-82.773
600	689.369	966.110	691.606	164.702	452.596	859.694	-74.841
700	755.691	1077.553	738.864	237.082	448.283	927.912	-69.240
800	808.745	1182.052	787.803	315.399	445.346	996.635	-65.072
900	851.851	1279.882	837.103	398.501	443.605	1065.646	-61.847
1000	887.357	1371.530	886.013	485.517	442.899	1134.808	-59.275
1100	916.929	1457.532	934.101	575.775	443.025	1204.009	-57.172
1200	941.780	1538.412	981.124	668.746	443.842	1273.148	-55.418
1300	962.824	1614.648	1026.953	764.004	445.163	1342.209	-53.930
1400	980.761	1686.675	1071.527	861.207	446.853	1411.158	-52.650
1500	996.143	1754.878	1114.831	960.071	448.834	1479.979	-51.536
1600	1009.407	1819.602	1156.873	1060.365	450.969	1548.650	-50.557
1700	1020.905	1881.150	1197.683	1161.894	453.186	1617.160	-49.688
1800	1030.923	1939.793	1237.295	1264.497	455.407	1685.608	-48.914
1900	1039.692	1995.772	1275.753	1368.037	457.601	1753.876	-48.216
2000	1047.402	2049.302	1313.102	1472.400	459.714	1822.059	-47.586
2100	1054.211	2100.573	1349.388	1577.487	461.664	1890.124	-47.013
2200	1060.248	2149.757	1384.658	1683.216	463.451	1958.103	-46.490
2300	1065.622	2197.007	1418.957	1789.515	465.071	2026.004	-46.011
2400	1070.423	2242.463	1452.329	1896.322	466.450	2093.786	-45.569
2500	1074.728	2286.249	1484.816	2003.583	467.601	2161.639	-45.164
2600	1078.600	2328.477	1516.457	2111.253	468.487	2229.324	-44.787
2700	1082.095	2369.251	1547.291	2219.290	469.113	2297.060	-44.438
2800	1085.258	2408.662	1577.355	2327.661	469.451	2364.799	-44.115
2900	1088.130	2446.796	1606.681	2436.332	469.471	2432.475	-43.813
3000	1090.743	2483.730	1635.304	2545.278	469.220	2500.185	-43.531
3100	1093.129	2519.535	1663.253	2654.473	468.616	2567.822	-43.267
3200	1095.311	2554.275	1690.557	2763.897	467.703	2635.565	-43.020
3300	1097.312	2588.011	1717.244	2873.530	466.464	2703.386	-42.790
3400	1099.151	2620.796	1743.339	2983.354	464.866	2771.153	-42.573
3500	1100.845	2652.683	1768.867	3093.355	462.917	2838.952	-42.368
3600	1102.408	2683.717	1793.851	3203.519	460.641	2906.910	-42.177
3700	1103.854	2713.942	1818.311	3313.833	458.003	2974.951	-41.998
3800	1105.194	2743.398	1842.270	3424.286	454.976	3043.006	-41.828
3900	1106.437	2772.122	1865.745	3534.868	451.605	3111.086	-41.667
4000	1107.593	2800.149	1888.756	3645.570	447.871	3179.411	-41.518
4100	1108.669	2827.512	1911.321	3756.384	443.736	3247.752	-41.376
4200	1109.673	2854.240	1933.454	3867.302	439.232	3316.189	-41.242
4300	1110.611	2880.362	1955.173	3978.316	434.343	3384.640	-41.114
4400	1111.488	2905.905	1976.491	4089.422	429.078	3453.308	-40.995
4500	1112.309	2930.893	1997.423	4200.612	423.455	3522.161	-40.883
4600	1113.080	2955.348	2017.983	4311.882	417.414	3591.155	-40.778
4700	1113.804	2979.294	2038.182	4423.227	410.975	3660.158	-40.677
4800	1114.485	3002.751	2058.034	4534.641	404.186	3729.419	-40.584
4900	1115.126	3025.738	2077.549	4646.122	396.967	3798.676	-40.494
5000	1115.730	3048.272	2096.739	4757.665	389.420	3868.288	-40.411

3.420. Benzo[de]naphtho[2,1,8,7-qrst]pentacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-83-8
Point Group: C_s

Length: 16.75 Å
Width: 10.79 Å
Breadth: 3.886 Å
L/B Ratio: 1.552

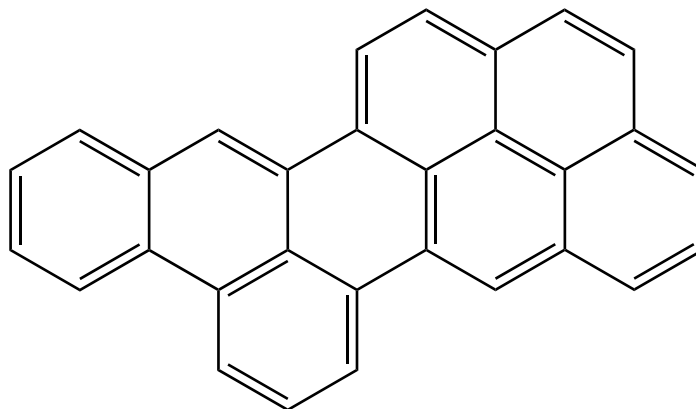
Cartesian coordinates:

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C	-5.8448	0.1847	0.0000	C	2.5895	1.9334	0.0000	H	-1.6352	3.4318	0.0000
C	-5.6655	-1.1734	0.0000	C	2.9521	-0.8684	0.0000	H	-3.9319	4.3785	0.0000
C	-4.3681	-1.7211	0.0000	C	1.6665	-0.3163	0.0000	H	-5.9123	2.8719	0.0000
C	-3.4191	0.5095	0.0000	C	0.5149	-1.1675	0.0000	H	-2.5941	-3.5129	0.0000
C	-2.2956	1.3894	0.0000	C	0.6886	-2.5667	0.0000	H	-0.3084	-4.4911	0.0000
C	-2.5026	2.7536	0.0000	C	2.0135	-3.1096	0.0000	H	0.0260	2.7301	0.0000
C	-3.8056	3.2908	0.0000	C	3.0980	-2.2928	0.0000	H	2.4627	3.0231	0.0000
C	-4.8956	2.4629	0.0000	C	3.9020	1.3944	0.0000	H	2.1300	-4.1994	0.0000
C	-4.7219	1.0528	0.0000	C	4.0930	-0.0033	0.0000	H	4.1211	-2.6996	0.0000
C	-1.9024	-1.4642	0.0000	C	5.4173	-0.5148	0.0000	H	5.5503	-1.6076	0.0000
C	-1.7076	-2.8596	0.0000	C	6.4941	0.3309	0.0000	H	7.5137	-0.0679	0.0000
C	-0.4436	-3.4036	0.0000	C	6.3009	1.7305	0.0000	H	7.1748	2.3901	0.0000
C	-0.9445	0.8295	0.0000	C	5.0352	2.2524	0.0000	H	4.8771	3.3369	0.0000
C	-0.7932	-0.6141	0.0000	H	-6.8512	0.6183	0.0000				
C	0.1512	1.6347	0.0000	H	-6.5277	-1.8484	0.0000				

Table 3.420: Table of thermodynamic data as a function of temperature for Benzo[de]naphtho[2,1,8,7-qrst]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-54.061	481.030	481.030	∞
100	116.224	368.285	837.074	-46.879	507.625	554.234	-289.496
200	234.621	483.188	631.317	-29.626	493.547	606.460	-158.388
250	303.008	542.839	607.623	-16.196	486.928	635.453	-132.768
298.15	369.549	601.913	601.913	0.000	481.030	664.609	-116.434
300	372.074	604.207	601.920	0.686	480.812	665.746	-115.914
350	438.489	666.600	606.696	20.966	475.371	697.012	-104.021
400	500.134	729.237	618.100	44.455	470.643	728.995	-95.195
450	556.032	791.430	633.911	70.884	466.544	761.540	-88.395
500	606.031	852.652	652.734	99.959	462.984	794.535	-83.003
600	689.884	970.861	695.991	164.922	457.174	861.421	-74.992
700	756.119	1082.377	743.307	237.349	452.908	929.160	-69.333
800	809.117	1186.929	792.297	315.706	450.010	997.398	-65.122
900	852.185	1284.800	841.642	398.843	448.305	1065.919	-61.863
1000	887.664	1376.482	890.591	485.891	447.631	1134.587	-59.264
1100	917.213	1462.513	938.714	576.178	447.787	1203.292	-57.138
1200	942.045	1543.416	985.769	669.176	448.631	1271.931	-55.365
1300	963.071	1619.673	1031.626	764.461	449.977	1340.491	-53.860
1400	980.991	1691.717	1076.226	861.687	451.691	1408.937	-52.567
1500	996.357	1759.936	1119.553	960.574	453.694	1477.252	-51.441
1600	1009.607	1824.673	1161.618	1060.888	455.850	1545.417	-50.452
1700	1021.092	1886.233	1202.446	1162.437	458.087	1613.419	-49.573
1800	1031.097	1944.886	1242.077	1265.057	460.325	1681.359	-48.791
1900	1039.854	2000.874	1280.551	1368.614	462.537	1749.117	-48.086
2000	1047.553	2054.412	1317.916	1472.993	464.665	1816.789	-47.449
2100	1054.352	2105.690	1354.216	1578.095	466.629	1884.343	-46.870
2200	1060.380	2154.880	1389.500	1683.838	468.430	1951.809	-46.341
2300	1065.746	2202.137	1423.811	1790.149	470.063	2019.199	-45.856
2400	1070.539	2247.598	1457.195	1896.968	471.454	2086.467	-45.410
2500	1074.837	2291.388	1489.692	2004.240	472.617	2153.806	-45.000
2600	1078.703	2333.621	1521.343	2111.921	473.513	2220.977	-44.619
2700	1082.192	2374.398	1552.187	2219.968	474.149	2288.198	-44.267
2800	1085.349	2413.812	1582.260	2328.348	474.496	2355.423	-43.940
2900	1088.216	2451.950	1611.595	2437.028	474.525	2422.584	-43.635
3000	1090.824	2488.886	1640.226	2545.982	474.283	2489.777	-43.350
3100	1093.205	2524.694	1668.182	2655.186	473.686	2556.899	-43.083
3200	1095.383	2559.437	1695.494	2764.617	472.781	2624.127	-42.834
3300	1097.381	2593.174	1722.188	2874.256	471.549	2691.431	-42.601
3400	1099.216	2625.962	1748.289	2984.088	469.958	2758.681	-42.381
3500	1100.907	2657.850	1773.823	3094.095	468.015	2825.964	-42.174
3600	1102.468	2688.886	1798.812	3204.265	465.745	2893.405	-41.981
3700	1103.911	2719.112	1823.279	3314.585	463.113	2960.929	-41.800
3800	1105.247	2748.570	1847.243	3425.043	460.091	3028.467	-41.628
3900	1106.488	2777.295	1870.723	3535.631	456.725	3096.029	-41.466
4000	1107.642	2805.324	1893.739	3646.338	452.996	3163.837	-41.315
4100	1108.716	2832.688	1916.308	3757.156	448.867	3231.660	-41.171
4200	1109.718	2859.417	1938.446	3868.079	444.367	3299.580	-41.035
4300	1110.653	2885.541	1960.169	3979.098	439.482	3367.513	-40.906
4400	1111.529	2911.084	1981.492	4090.207	434.222	3435.663	-40.786
4500	1112.349	2936.073	2002.428	4201.402	428.602	3503.998	-40.673
4600	1113.118	2960.529	2022.991	4312.675	422.566	3572.474	-40.566
4700	1113.841	2984.476	2043.194	4424.024	416.130	3640.959	-40.464
4800	1114.520	3007.933	2063.050	4535.442	409.344	3709.702	-40.369
4900	1115.160	3030.921	2082.568	4646.926	402.129	3778.441	-40.278
5000	1115.762	3053.456	2101.762	4758.473	394.585	3847.535	-40.194

3.421. Benzo[qr]naphtho[2,1,8,7-defg]pentacene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-67-8
Point Group: C_s

Length: 16.59 Å
Width: 10.33 Å
Breadth: 3.888 Å
L/B Ratio: 1.606

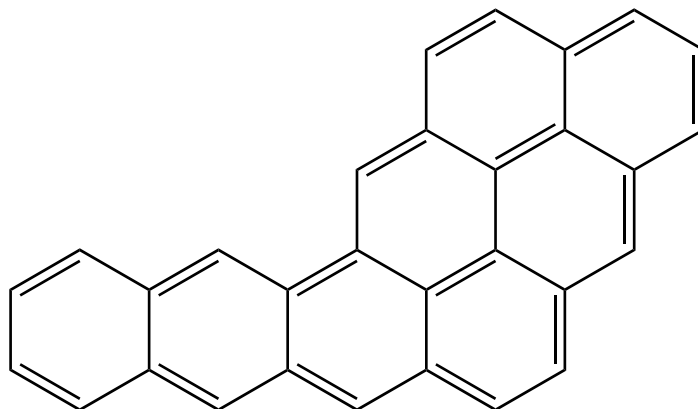
Cartesian coordinates:

C	1.4301	-0.7399	0.0000	C	-5.6208	1.8194	0.0000	H	2.2837	4.5345	0.0000
C	2.4957	-1.5941	0.0000	C	-5.8522	0.4486	0.0000	H	-0.0436	3.6598	0.0000
C	0.5595	1.5932	0.0000	C	-2.3443	-0.8471	0.0000	H	-1.6627	-4.1992	0.0000
C	1.6504	0.6861	0.0000	C	-3.4572	0.0543	0.0000	H	0.6578	-3.3174	0.0000
C	2.9666	1.1873	0.0000	C	-4.7787	-0.4470	0.0000	H	-1.7186	3.0243	0.0000
C	3.1797	2.5815	0.0000	C	-4.9838	-1.8728	0.0000	H	-4.1555	3.4043	0.0000
C	2.1145	3.4527	0.0000	C	-3.9344	-2.7265	0.0000	H	-6.4698	2.5113	0.0000
C	0.8054	2.9589	0.0000	C	-2.5789	-2.2400	0.0000	H	-6.8787	0.0648	0.0000
C	0.0576	-1.2442	0.0000	C	4.0861	0.2721	0.0000	H	-6.0149	-2.2443	0.0000
C	-1.4889	-3.1171	0.0000	C	3.8418	-1.1116	0.0000	H	-4.0899	-3.8116	0.0000
C	-0.1962	-2.6222	0.0000	C	4.9289	-2.0144	0.0000	H	4.7287	-3.0919	0.0000
C	-1.0213	-0.3451	0.0000	C	6.2213	-1.5436	0.0000	H	7.0647	-2.2418	0.0000
C	-0.8133	1.0861	0.0000	C	6.4690	-0.1601	0.0000	H	7.5021	0.2024	0.0000
C	-1.8816	1.9343	0.0000	C	5.4213	0.7314	0.0000	H	5.6025	1.8171	0.0000
C	-3.2321	1.4488	0.0000	H	2.3276	-2.6834	0.0000				
C	-4.3256	2.3218	0.0000	H	4.2152	2.9551	0.0000				

Table 3.421: Table of thermodynamic data as a function of temperature for Benzo[*qr*]naphtho[2,1,8,7-*defg*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-54.106	472.033	472.033	∞
100	116.400	373.129	841.949	-46.882	498.625	544.749	-284.542
200	234.645	488.140	636.211	-29.614	484.560	596.484	-155.782
250	302.880	547.779	612.528	-16.187	477.939	625.230	-130.632
298.15	369.324	606.821	606.821	0.000	472.033	654.148	-114.602
300	371.846	609.114	606.828	0.686	471.814	655.276	-114.091
350	438.213	671.468	611.601	20.953	466.360	686.297	-102.422
400	499.844	734.067	622.998	44.427	461.618	718.038	-93.764
450	555.748	796.226	638.799	70.842	457.504	750.343	-87.096
500	605.763	857.419	657.611	99.904	453.930	783.099	-81.808
600	689.659	975.583	700.846	164.842	448.096	849.510	-73.955
700	755.934	1087.067	748.140	237.249	443.809	916.779	-68.409
800	808.966	1191.597	797.111	315.589	440.895	984.549	-64.283
900	852.063	1289.452	846.439	398.712	439.176	1052.604	-61.090
1000	887.563	1381.122	895.373	485.749	438.491	1120.808	-58.544
1100	917.130	1467.144	943.483	576.027	438.638	1189.049	-56.462
1200	941.975	1548.040	990.526	669.017	439.474	1257.226	-54.724
1300	963.012	1624.292	1036.373	764.295	440.814	1325.323	-53.251
1400	980.941	1696.332	1080.964	861.516	442.523	1393.307	-51.984
1500	996.314	1764.548	1124.282	960.398	444.521	1461.161	-50.881
1600	1009.569	1829.282	1166.339	1060.709	446.673	1528.865	-49.911
1700	1021.059	1890.840	1207.161	1162.254	448.906	1596.407	-49.051
1800	1031.068	1949.492	1246.785	1264.871	451.142	1663.885	-48.284
1900	1039.828	2005.478	1285.254	1368.426	453.350	1731.183	-47.593
2000	1047.530	2059.015	1322.614	1472.802	455.476	1798.395	-46.968
2100	1054.332	2110.292	1358.910	1577.902	457.438	1865.489	-46.401
2200	1060.362	2159.481	1394.189	1683.642	459.237	1932.495	-45.882
2300	1065.729	2206.737	1428.497	1789.952	460.868	1999.424	-45.407
2400	1070.524	2252.197	1461.877	1896.769	462.258	2066.233	-44.969
2500	1074.823	2295.987	1494.371	2004.040	463.419	2133.112	-44.568
2600	1078.690	2338.219	1526.019	2111.719	464.314	2199.822	-44.194
2700	1082.180	2378.995	1556.860	2219.766	464.948	2266.584	-43.849
2800	1085.338	2418.410	1586.930	2328.144	465.295	2333.349	-43.528
2900	1088.206	2456.546	1616.262	2436.824	465.322	2400.050	-43.229
3000	1090.815	2493.483	1644.891	2545.777	465.079	2466.784	-42.950
3100	1093.197	2529.290	1672.845	2654.979	464.482	2533.446	-42.687
3200	1095.375	2564.033	1700.155	2764.409	463.576	2600.214	-42.443
3300	1097.373	2597.770	1726.846	2874.048	462.343	2667.059	-42.215
3400	1099.209	2630.558	1752.946	2983.879	460.751	2733.850	-42.000
3500	1100.901	2662.446	1778.478	3093.885	458.808	2800.673	-41.797
3600	1102.461	2693.481	1803.466	3204.054	456.537	2867.654	-41.608
3700	1103.905	2723.707	1827.931	3314.374	453.904	2934.719	-41.430
3800	1105.242	2753.165	1851.893	3424.832	450.882	3001.797	-41.262
3900	1106.483	2781.890	1875.372	3535.419	447.515	3068.900	-41.102
4000	1107.637	2809.918	1898.387	3646.125	443.786	3136.248	-40.954
4100	1108.711	2837.282	1920.955	3756.943	439.656	3203.612	-40.814
4200	1109.713	2864.012	1943.091	3867.865	435.156	3271.073	-40.681
4300	1110.649	2890.135	1964.813	3978.884	430.270	3338.546	-40.554
4400	1111.525	2915.678	1986.134	4089.993	425.009	3406.237	-40.436
4500	1112.345	2940.667	2007.070	4201.187	419.389	3474.112	-40.326
4600	1113.114	2965.123	2027.632	4312.460	413.353	3542.129	-40.221
4700	1113.837	2989.070	2047.834	4423.808	406.917	3610.155	-40.122
4800	1114.517	3012.527	2067.689	4535.226	400.131	3678.438	-40.029
4900	1115.156	3035.514	2087.206	4646.710	392.915	3746.717	-39.940
5000	1115.759	3058.050	2106.399	4758.256	385.371	3815.352	-39.858

3.422. Naphtho[3,2,1,8,7-vwxyz]hexaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-85-0
Point Group: C_s

Length: 18.02 Å
Width: 10.44 Å
Breadth: 3.886 Å
L/B Ratio: 1.726

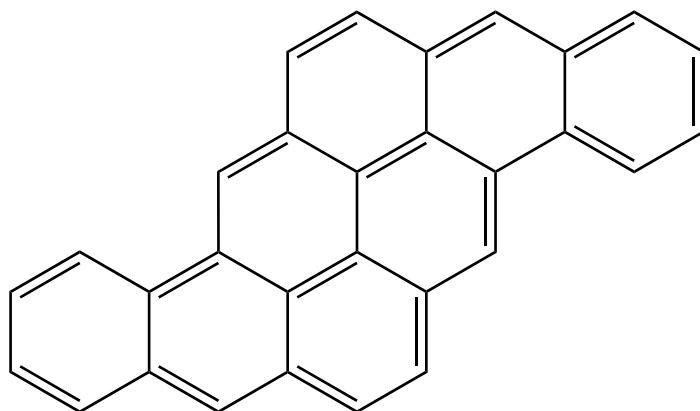
Cartesian coordinates:

C	6.5272	-1.9481	0.0000	C	0.6242	-0.1735	0.0000	H	6.7126	1.4678	0.0000
C	7.0906	-0.6428	0.0000	C	-0.1835	0.9772	0.0000	H	4.7319	-3.1206	0.0000
C	6.2871	0.4579	0.0000	C	-1.5913	0.8514	0.0000	H	4.4543	2.4400	0.0000
C	5.1749	-2.1184	0.0000	C	0.0229	-1.4456	0.0000	H	2.4659	-2.1461	0.0000
C	4.3040	-0.9857	0.0000	C	-4.4150	0.5975	0.0000	H	2.2368	3.4217	0.0000
C	4.8651	0.3150	0.0000	C	-5.8119	0.4496	0.0000	H	0.0142	4.4385	0.0000
C	4.0172	1.4337	0.0000	C	-6.3802	-0.8128	0.0000	H	-2.4483	4.2052	0.0000
C	2.9083	-1.1369	0.0000	C	-5.5817	-1.9573	0.0000	H	-4.4437	2.7763	0.0000
C	2.0689	-0.0301	0.0000	C	-1.3565	-1.5845	0.0000	H	0.6733	-2.3351	0.0000
C	2.6352	1.2767	0.0000	C	-2.1781	-0.4253	0.0000	H	-6.4482	1.3418	0.0000
C	1.7734	2.4271	0.0000	C	-3.6013	-0.5572	0.0000	H	-7.4703	-0.9184	0.0000
C	0.4182	2.2910	0.0000	C	-4.1935	-1.8438	0.0000	H	-6.0482	-2.9489	0.0000
C	-0.4586	3.4492	0.0000	C	-3.3353	-3.0053	0.0000	H	-3.8122	-3.9922	0.0000
C	-1.7973	3.3230	0.0000	C	-1.9900	-2.8825	0.0000	H	-1.3424	-3.7668	0.0000
C	-2.4365	2.0194	0.0000	H	7.1994	-2.8123	0.0000				
C	-3.7974	1.8899	0.0000	H	8.1806	-0.5393	0.0000				

Table 3.422: Table of thermodynamic data as a function of temperature for Naphtho[3,2,1,8,7-*vwxyz*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.650	474.912	474.912	∞
100	113.889	360.719	827.536	-46.682	501.705	549.070	-286.799
200	233.814	474.483	622.401	-29.584	487.471	602.125	-157.256
250	302.630	534.005	598.735	-16.182	480.824	631.558	-131.954
298.15	369.329	593.029	593.029	0.000	474.912	661.140	-115.827
300	371.857	595.322	593.036	0.686	474.694	662.294	-115.313
350	438.273	657.683	597.810	20.956	469.242	694.004	-103.572
400	499.858	720.287	609.208	44.432	464.502	726.434	-94.861
450	555.689	782.444	625.010	70.845	460.388	759.428	-88.150
500	605.639	843.627	643.823	99.902	456.809	792.873	-82.829
600	689.469	961.761	687.055	164.824	450.958	860.665	-74.926
700	755.754	1073.216	734.342	237.212	446.652	929.317	-69.345
800	808.833	1177.725	783.305	315.536	443.722	998.474	-65.192
900	851.988	1275.568	832.625	398.649	441.993	1067.916	-61.979
1000	887.542	1367.232	881.551	485.681	441.303	1137.509	-59.416
1100	917.153	1453.255	929.655	575.960	441.450	1207.139	-57.321
1200	942.033	1534.155	976.693	668.954	442.290	1276.705	-55.572
1300	963.094	1610.412	1022.536	764.239	443.637	1346.191	-54.089
1400	981.040	1682.459	1067.124	861.469	445.356	1415.562	-52.814
1500	996.424	1750.682	1110.441	960.362	447.364	1484.803	-51.704
1600	1009.686	1815.423	1152.496	1060.683	449.528	1553.893	-50.728
1700	1021.178	1876.988	1193.318	1162.240	451.772	1622.820	-49.862
1800	1031.187	1935.647	1232.942	1264.870	454.020	1691.684	-49.090
1900	1039.946	1991.640	1271.411	1368.436	456.240	1760.365	-48.395
2000	1047.646	2045.183	1308.771	1472.824	458.378	1828.961	-47.767
2100	1054.444	2096.465	1345.068	1577.935	460.351	1897.438	-47.195
2200	1060.471	2145.660	1380.348	1683.687	462.161	1965.826	-46.674
2300	1065.834	2192.920	1414.656	1790.007	463.803	2034.137	-46.196
2400	1070.625	2238.385	1448.037	1896.834	465.203	2102.327	-45.755
2500	1074.920	2282.179	1480.532	2004.116	466.374	2170.588	-45.351
2600	1078.783	2324.414	1512.182	2111.804	467.278	2238.679	-44.975
2700	1082.268	2365.194	1543.024	2219.860	467.922	2306.821	-44.627
2800	1085.423	2404.612	1573.095	2328.247	468.277	2374.966	-44.305
2900	1088.286	2442.751	1602.429	2436.934	468.313	2443.046	-44.003
3000	1090.892	2479.691	1631.059	2545.895	468.078	2511.160	-43.722
3100	1093.270	2515.500	1659.015	2655.105	467.488	2579.201	-43.458
3200	1095.446	2550.245	1686.325	2764.543	466.589	2647.348	-43.213
3300	1097.441	2583.985	1713.018	2874.188	465.363	2715.571	-42.983
3400	1099.274	2616.774	1739.120	2984.025	463.778	2783.740	-42.766
3500	1100.962	2648.664	1764.653	3094.038	461.841	2851.942	-42.562
3600	1102.520	2679.701	1789.642	3204.213	459.576	2920.301	-42.372
3700	1103.961	2709.929	1814.108	3314.538	456.949	2988.744	-42.193
3800	1105.296	2739.388	1838.071	3425.002	453.933	3057.200	-42.023
3900	1106.535	2768.114	1861.552	3535.594	450.571	3125.680	-41.863
4000	1107.686	2796.144	1884.568	3646.306	446.847	3194.406	-41.714
4100	1108.759	2823.509	1907.136	3757.129	442.721	3263.147	-41.572
4200	1109.759	2850.240	1929.274	3868.056	438.226	3331.985	-41.438
4300	1110.693	2876.364	1950.997	3979.079	433.345	3400.835	-41.311
4400	1111.567	2901.908	1972.319	4090.192	428.089	3469.904	-41.192
4500	1112.386	2926.898	1993.255	4201.390	422.473	3539.156	-41.081
4600	1113.154	2951.355	2013.819	4312.668	416.440	3608.549	-40.976
4700	1113.875	2975.303	2034.022	4424.019	410.008	3677.952	-40.875
4800	1114.553	2998.761	2053.877	4535.441	403.226	3747.612	-40.781
4900	1115.191	3021.749	2073.396	4646.929	396.013	3817.268	-40.692
5000	1115.793	3044.285	2092.589	4758.478	388.473	3887.279	-40.609

3.423. Pyranthrene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 191-13-9
Point Group: C_{2h}

Length: 18.01 Å
Width: 10.44 Å
Breadth: 3.889 Å
L/B Ratio: 1.726

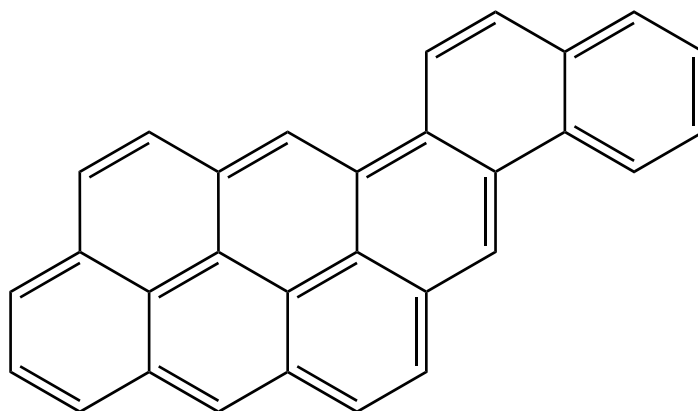
Cartesian coordinates:

C	6.0821	-1.5987	0.0000	C	-2.4887	0.5454	0.0000	H	6.4851	1.7888	0.0000
C	6.7273	-0.3455	0.0000	C	-3.8067	-1.9611	0.0000	H	4.1930	-2.6413	0.0000
C	5.9897	0.8111	0.0000	C	-0.3349	-0.6168	0.0000	H	4.3348	2.9228	0.0000
C	4.7120	-1.6705	0.0000	C	-1.7580	-0.6526	0.0000	H	2.1775	4.0866	0.0000
C	3.9264	-0.4923	0.0000	C	-2.4366	-1.9176	0.0000	H	-0.2979	4.0122	0.0000
C	4.5728	0.7593	0.0000	C	-1.6413	-3.1302	0.0000	H	-2.3926	2.7109	0.0000
C	3.8068	1.9611	0.0000	C	-0.2953	-3.0904	0.0000	H	2.3928	-2.7108	0.0000
C	2.4366	1.9177	0.0000	C	0.4214	-1.8310	0.0000	H	-4.3347	-2.9228	0.0000
C	1.6414	3.1303	0.0000	C	-4.5728	-0.7593	0.0000	H	-2.1774	-4.0865	0.0000
C	0.2954	3.0904	0.0000	C	-3.9264	0.4924	0.0000	H	0.2980	-4.0121	0.0000
C	-0.4213	1.8311	0.0000	C	-4.7122	1.6705	0.0000	H	-4.1934	2.6413	0.0000
C	-1.7963	1.7842	0.0000	C	-6.0823	1.5985	0.0000	H	-6.6853	2.5124	0.0000
C	1.7580	0.6527	0.0000	C	-6.7274	0.3453	0.0000	H	-7.8216	0.3059	0.0000
C	0.3350	0.6169	0.0000	C	-5.9897	-0.8113	0.0000	H	-6.4850	-1.7890	0.0000
C	1.7964	-1.7841	0.0000	H	6.6849	-2.5127	0.0000				
C	2.4887	-0.5453	0.0000	H	7.8215	-0.3063	0.0000				

Table 3.423: Table of thermodynamic data as a function of temperature for Pyranthrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-53.624	468.032	468.032	∞
100	114.289	350.962	818.214	-46.725	494.781	543.122	-283.692
200	233.987	464.986	612.942	-29.591	480.583	597.137	-155.953
250	302.683	524.531	589.271	-16.185	473.941	627.043	-131.011
298.15	369.397	583.564	583.564	0.000	468.032	657.082	-115.116
300	371.927	585.857	583.571	0.686	467.814	658.253	-114.610
350	438.430	648.235	588.346	20.961	462.368	690.436	-103.040
400	500.110	710.867	599.748	44.448	457.638	723.338	-94.456
450	556.017	773.057	615.556	70.876	453.538	756.802	-87.845
500	606.017	834.278	634.377	99.951	449.977	790.716	-82.604
600	689.878	952.485	677.631	164.912	444.167	859.439	-74.819
700	756.136	1064.002	724.945	237.340	439.900	929.016	-69.323
800	809.165	1168.558	773.933	315.700	437.006	999.091	-65.233
900	852.264	1266.437	823.278	398.843	435.307	1069.448	-62.068
1000	887.768	1358.128	872.228	485.900	434.642	1139.953	-59.544
1100	917.336	1444.170	920.352	576.199	434.809	1210.492	-57.480
1200	942.180	1525.084	967.409	669.210	435.666	1280.965	-55.758
1300	963.212	1601.352	1013.269	764.508	437.027	1351.358	-54.297
1400	981.135	1673.407	1057.872	861.749	438.755	1421.635	-53.041
1500	996.501	1741.636	1101.202	960.650	440.772	1491.781	-51.947
1600	1009.748	1806.382	1143.270	1060.979	442.943	1561.775	-50.986
1700	1021.229	1867.950	1184.102	1162.541	445.193	1631.606	-50.132
1800	1031.229	1926.611	1223.736	1265.175	447.445	1701.374	-49.372
1900	1039.981	1982.607	1262.214	1368.745	449.669	1770.959	-48.686
2000	1047.674	2036.150	1299.582	1473.136	451.810	1840.458	-48.067
2100	1054.468	2087.434	1335.887	1578.250	453.786	1909.837	-47.504
2200	1060.490	2136.630	1371.174	1684.004	455.598	1979.129	-46.990
2300	1065.850	2183.891	1405.488	1790.326	457.242	2048.343	-46.518
2400	1070.638	2229.356	1438.875	1897.155	458.643	2117.436	-46.084
2500	1074.931	2273.151	1471.376	2004.437	459.815	2186.599	-45.686
2600	1078.792	2315.387	1503.030	2112.127	460.721	2255.593	-45.314
2700	1082.276	2356.167	1533.877	2220.183	461.365	2324.638	-44.972
2800	1085.430	2395.585	1563.952	2328.571	461.721	2393.685	-44.654
2900	1088.292	2433.725	1593.290	2437.259	461.758	2462.668	-44.357
3000	1090.897	2470.664	1621.924	2546.221	461.523	2531.685	-44.080
3100	1093.274	2506.474	1649.883	2655.431	460.933	2600.628	-43.819
3200	1095.449	2541.219	1677.197	2764.869	460.035	2669.678	-43.577
3300	1097.443	2574.958	1703.893	2874.515	458.809	2738.804	-43.351
3400	1099.276	2607.748	1729.997	2984.352	457.224	2807.876	-43.137
3500	1100.964	2639.638	1755.534	3094.365	455.288	2876.980	-42.936
3600	1102.522	2670.675	1780.525	3204.541	453.023	2946.242	-42.748
3700	1103.962	2700.903	1804.993	3314.866	450.396	3015.587	-42.572
3800	1105.297	2730.362	1828.959	3425.330	447.380	3084.946	-42.405
3900	1106.535	2759.089	1852.442	3535.922	444.018	3154.329	-42.247
4000	1107.687	2787.118	1875.460	3646.634	440.294	3223.957	-42.100
4100	1108.759	2814.483	1898.030	3757.457	436.169	3293.601	-41.960
4200	1109.759	2841.214	1920.170	3868.383	431.673	3363.341	-41.828
4300	1110.693	2867.338	1941.895	3979.406	426.793	3433.094	-41.703
4400	1111.567	2892.883	1963.219	4090.520	421.536	3503.065	-41.586
4500	1112.386	2917.872	1984.157	4201.718	415.920	3573.220	-41.476
4600	1113.154	2942.329	2004.722	4312.995	409.888	3643.516	-41.373
4700	1113.875	2966.277	2024.926	4424.347	403.455	3713.821	-41.274
4800	1114.553	2989.735	2044.783	4535.769	396.673	3784.384	-41.182
4900	1115.191	3012.723	2064.303	4647.256	389.461	3854.942	-41.093
5000	1115.793	3035.259	2083.498	4758.806	381.920	3925.856	-41.012

3.424. Benzo[*c*]naphtho[7,8,1,2,3-*pqrst*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-80-5
Point Group: C_s

Length: 17.94 Å
Width: 10.36 Å
Breadth: 3.885 Å
L/B Ratio: 1.732

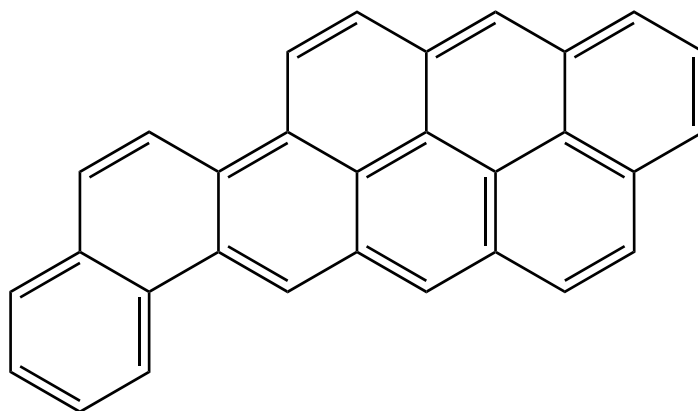
Cartesian coordinates:

C	5.8890	-1.2312	0.0000	C	1.6703	-1.6880	0.0000	H	6.1025	2.1749	0.0000
C	6.4523	0.0501	0.0000	C	2.5488	-2.8378	0.0000	H	3.8569	3.1919	0.0000
C	5.6530	1.1755	0.0000	C	3.8907	-2.6961	0.0000	H	1.6162	4.2033	0.0000
C	4.2492	1.0506	0.0000	C	4.5093	-1.3887	0.0000	H	-0.8460	3.9459	0.0000
C	3.3969	2.1960	0.0000	C	-1.9798	-0.8138	0.0000	H	-2.8359	2.5044	0.0000
C	2.0329	2.0582	0.0000	C	-2.7819	0.3344	0.0000	H	-0.1658	-2.8204	0.0000
C	1.1522	3.2102	0.0000	C	-3.9486	-2.2385	0.0000	H	2.0863	-3.8316	0.0000
C	-0.1869	3.0699	0.0000	C	-2.5984	-2.1048	0.0000	H	4.5508	-3.5712	0.0000
C	-0.8125	1.7619	0.0000	C	-4.7947	-1.0840	0.0000	H	-4.4165	-3.2297	0.0000
C	-2.1784	1.6201	0.0000	C	-4.2198	0.1997	0.0000	H	-1.9410	-2.9879	0.0000
C	1.4369	0.7499	0.0000	C	-5.0721	1.3286	0.0000	H	-4.6154	2.3300	0.0000
C	0.0240	0.6009	0.0000	C	-6.4375	1.1768	0.0000	H	-7.0911	2.0552	0.0000
C	-0.5500	-0.6854	0.0000	C	-7.0083	-0.1093	0.0000	H	-8.0982	-0.2140	0.0000
C	0.2983	-1.8212	0.0000	C	-6.2022	-1.2219	0.0000	H	-6.6388	-2.2271	0.0000
C	3.6760	-0.2399	0.0000	H	6.5411	-2.1120	0.0000				
C	2.2568	-0.3858	0.0000	H	7.5425	0.1552	0.0000				

Table 3.424: Table of thermodynamic data as a function of temperature for Benzo[*c*]naphtho[7,8,1,2,3-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.651	465.226	465.226	∞
100	114.343	361.112	827.613	-46.650	492.050	539.376	-281.735
200	233.597	474.968	622.682	-29.543	477.825	592.383	-154.711
250	302.196	534.417	599.050	-16.158	471.162	621.792	-129.914
298.15	368.767	593.353	593.353	0.000	465.226	651.357	-114.113
300	371.291	595.641	593.360	0.685	465.006	652.510	-113.610
350	437.650	657.911	598.126	20.925	459.524	684.207	-102.110
400	499.224	720.431	609.508	44.369	454.753	716.628	-93.580
450	555.071	782.513	625.288	70.751	450.607	749.616	-87.011
500	605.048	843.633	644.076	99.778	446.998	783.060	-81.804
600	688.934	961.664	687.258	164.644	441.091	850.857	-74.072
700	755.261	1073.040	734.497	236.980	436.734	919.523	-68.614
800	808.371	1177.485	783.414	315.256	433.756	988.700	-64.554
900	851.549	1275.274	832.692	398.324	431.982	1058.169	-61.413
1000	887.124	1366.894	881.580	485.313	431.249	1127.793	-58.909
1100	916.757	1452.877	929.649	575.551	431.355	1197.460	-56.861
1200	941.658	1533.744	976.654	668.507	432.157	1267.064	-55.153
1300	962.740	1609.972	1022.468	763.756	433.468	1336.593	-53.704
1400	980.708	1681.994	1067.028	860.952	435.152	1406.010	-52.458
1500	996.113	1750.194	1110.320	959.812	437.128	1475.298	-51.373
1600	1009.394	1814.916	1152.352	1060.104	439.261	1544.438	-50.420
1700	1020.906	1876.464	1193.151	1161.632	441.478	1613.417	-49.573
1800	1030.933	1935.108	1232.755	1264.235	443.699	1682.334	-48.819
1900	1039.708	1991.088	1271.205	1367.777	445.895	1751.070	-48.139
2000	1047.424	2044.618	1308.547	1472.142	448.010	1819.721	-47.525
2100	1054.236	2095.890	1344.828	1577.232	449.961	1888.255	-46.967
2200	1060.276	2145.076	1380.092	1682.963	451.751	1956.702	-46.457
2300	1065.651	2192.328	1414.386	1789.265	453.374	2025.071	-45.990
2400	1070.454	2237.785	1447.754	1896.074	454.756	2093.321	-45.559
2500	1074.759	2281.572	1480.236	2003.339	455.911	2161.642	-45.164
2600	1078.631	2323.801	1511.874	2111.012	456.800	2229.794	-44.796
2700	1082.126	2364.576	1542.704	2219.053	457.428	2297.998	-44.457
2800	1085.288	2403.988	1572.765	2327.426	457.770	2366.205	-44.141
2900	1088.159	2442.123	1602.089	2436.100	457.792	2434.348	-43.846
3000	1090.772	2479.058	1630.708	2545.049	457.545	2502.524	-43.572
3100	1093.157	2514.864	1658.655	2654.247	456.943	2570.629	-43.314
3200	1095.338	2549.605	1685.957	2763.674	456.033	2638.839	-43.074
3300	1097.338	2583.342	1712.642	2873.309	454.797	2707.127	-42.849
3400	1099.177	2616.128	1738.735	2983.136	453.202	2775.361	-42.637
3500	1100.870	2648.015	1764.261	3093.139	451.255	2843.627	-42.438
3600	1102.433	2679.050	1789.243	3203.306	448.981	2912.051	-42.252
3700	1103.878	2709.275	1813.702	3313.622	446.346	2980.559	-42.077
3800	1105.216	2738.732	1837.659	3424.078	443.321	3049.081	-41.912
3900	1106.459	2767.457	1861.133	3534.662	439.952	3117.627	-41.755
4000	1107.614	2795.485	1884.143	3645.366	436.220	3186.418	-41.609
4100	1108.689	2822.848	1906.706	3756.182	432.088	3255.226	-41.471
4200	1109.692	2849.577	1928.838	3867.102	427.586	3324.130	-41.341
4300	1110.630	2875.699	1950.556	3978.118	422.698	3393.046	-41.216
4400	1111.506	2901.242	1971.873	4089.226	417.436	3462.181	-41.100
4500	1112.327	2926.230	1992.804	4200.418	411.814	3531.500	-40.992
4600	1113.097	2950.687	2013.363	4311.689	405.775	3600.960	-40.889
4700	1113.821	2974.633	2033.562	4423.036	399.338	3670.430	-40.791
4800	1114.501	2998.090	2053.412	4534.452	392.550	3740.157	-40.700
4900	1115.141	3021.077	2072.927	4645.935	385.332	3809.880	-40.613
5000	1115.745	3043.612	2092.116	4757.479	377.787	3879.958	-40.533

3.425. Phenanthro[2,3,4,5-*tuvab*]picene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 120835-81-6
Point Group: C_s

Length: 17.73 Å
Width: 10.23 Å
Breadth: 3.886 Å
L/B Ratio: 1.734

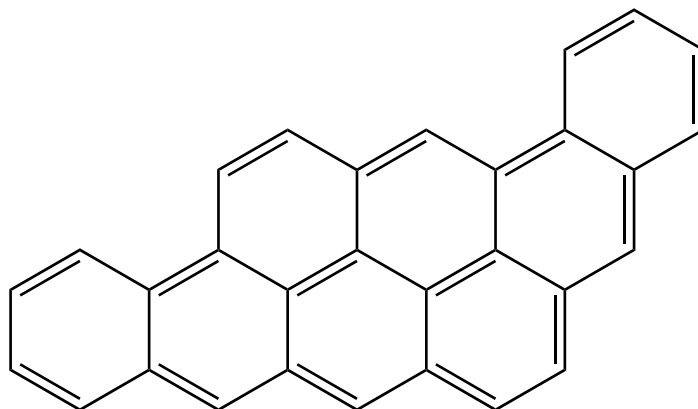
Cartesian coordinates:

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C	6.9144	1.0363	0.0000	C	-6.0306	1.0123	0.0000	H	3.9254	2.6881	0.0000
C	6.0038	2.1034	0.0000	C	-6.4814	-0.3195	0.0000	H	2.8865	-3.1794	0.0000
C	4.6480	1.8579	0.0000	C	-5.5900	-1.3657	0.0000	H	5.3240	-2.6965	0.0000
C	5.0721	-0.5293	0.0000	C	-2.3422	0.4880	0.0000	H	2.1650	2.3409	0.0000
C	4.1563	0.5366	0.0000	C	-3.7379	0.2185	0.0000	H	-0.1575	3.1403	0.0000
C	3.2622	-2.1447	0.0000	C	-4.1957	-1.1182	0.0000	H	-2.4841	3.9440	0.0000
C	4.5885	-1.8838	0.0000	C	-3.2543	-2.1804	0.0000	H	-4.9129	3.4611	0.0000
C	2.2872	-1.0858	0.0000	C	-0.0235	-0.3035	0.0000	H	-6.7607	1.8295	0.0000
C	2.7312	0.2589	0.0000	C	-1.4278	-0.5707	0.0000	H	-7.5589	-0.5158	0.0000
C	1.8005	1.3008	0.0000	C	-1.9010	-1.9212	0.0000	H	-5.9464	-2.4020	0.0000
C	0.4286	1.0420	0.0000	C	-0.9232	-2.9849	0.0000	H	-3.6208	-3.2143	0.0000
C	-0.5262	2.1071	0.0000	C	0.4001	-2.7190	0.0000	H	-1.2905	-4.0177	0.0000
C	-1.8704	1.8473	0.0000	C	0.9049	-1.3654	0.0000	H	1.1426	-3.5318	0.0000
C	-2.8544	2.9122	0.0000	H	7.1627	-1.1012	0.0000				
C	-4.1757	2.6498	0.0000	H	7.9895	1.2433	0.0000				

Table 3.425: Table of thermodynamic data as a function of temperature for Phenanthro[2,3,4,5-*tu**uvab*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-54.114	475.012	475.012	∞
100	115.496	363.444	833.697	-47.025	501.461	548.554	-286.529
200	235.522	478.311	627.149	-29.768	487.387	601.276	-157.034
250	304.510	538.233	603.340	-16.277	480.830	630.506	-131.734
298.15	371.354	597.601	597.601	0.000	475.012	659.877	-115.605
300	373.886	599.906	597.608	0.689	474.797	661.022	-115.092
350	440.403	662.589	602.407	21.064	469.450	692.495	-103.347
400	502.025	725.480	613.862	44.647	464.818	724.673	-94.631
450	557.836	787.891	629.738	71.169	460.811	757.400	-87.915
500	607.720	849.298	648.634	100.332	457.338	790.567	-82.588
600	691.337	967.794	692.041	165.452	451.686	857.773	-74.674
700	757.367	1079.518	739.498	238.014	447.554	925.808	-69.083
800	810.202	1184.225	788.617	316.487	444.773	994.324	-64.921
900	853.140	1282.217	838.078	399.725	443.169	1063.109	-61.700
1000	888.512	1373.993	887.130	486.863	442.585	1132.030	-59.130
1100	917.972	1460.100	935.345	577.231	442.821	1200.980	-57.029
1200	942.728	1541.066	982.482	670.301	443.737	1269.858	-55.274
1300	963.689	1617.375	1028.413	765.650	445.149	1338.650	-53.786
1400	981.552	1689.463	1073.081	862.936	446.922	1407.323	-52.507
1500	996.868	1757.719	1116.468	961.876	448.978	1475.862	-51.393
1600	1010.074	1822.487	1158.588	1062.239	451.183	1544.247	-50.413
1700	1021.520	1884.074	1199.467	1163.832	453.464	1612.466	-49.544
1800	1031.490	1942.751	1239.144	1266.494	455.744	1680.620	-48.769
1900	1040.216	1998.760	1277.661	1370.089	457.993	1748.591	-48.071
2000	1047.887	2052.315	1315.064	1474.502	460.156	1816.473	-47.440
2100	1054.661	2103.609	1351.401	1579.636	462.152	1884.236	-46.867
2200	1060.667	2152.813	1386.719	1685.409	463.983	1951.910	-46.343
2300	1066.012	2200.082	1421.061	1791.748	465.644	2019.505	-45.863
2400	1070.788	2245.554	1454.474	1898.592	467.060	2086.979	-45.421
2500	1075.069	2289.354	1486.998	2005.889	468.247	2154.522	-45.015
2600	1078.920	2331.595	1518.675	2113.592	469.166	2221.895	-44.637
2700	1082.395	2372.380	1549.543	2221.660	469.822	2289.319	-44.289
2800	1085.540	2411.802	1579.638	2330.059	470.190	2356.745	-43.965
2900	1088.395	2449.946	1608.995	2438.758	470.237	2424.106	-43.662
3000	1090.993	2486.889	1637.645	2547.730	470.012	2491.500	-43.380
3100	1093.364	2522.701	1665.621	2656.950	469.432	2558.821	-43.115
3200	1095.534	2557.449	1692.950	2766.396	468.542	2626.248	-42.868
3300	1097.523	2591.191	1719.661	2876.050	467.324	2693.751	-42.638
3400	1099.351	2623.983	1745.779	2985.895	465.747	2761.199	-42.420
3500	1101.035	2655.875	1771.328	3095.916	463.818	2828.679	-42.215
3600	1102.589	2686.914	1796.332	3206.098	461.560	2896.318	-42.024
3700	1104.026	2717.144	1820.812	3316.430	458.940	2964.039	-41.844
3800	1105.357	2746.604	1844.789	3426.900	455.930	3031.773	-41.674
3900	1106.593	2775.333	1868.282	3537.498	452.574	3099.532	-41.513
4000	1107.741	2803.364	1891.310	3648.215	448.855	3167.536	-41.363
4100	1108.811	2830.730	1913.890	3759.043	444.736	3235.555	-41.221
4200	1109.809	2857.462	1936.039	3869.975	440.245	3303.671	-41.086
4300	1110.740	2883.587	1957.773	3981.003	435.369	3371.799	-40.958
4400	1111.612	2909.133	1979.105	4092.121	430.117	3440.145	-40.839
4500	1112.429	2934.123	2000.051	4203.324	424.506	3508.674	-40.727
4600	1113.195	2958.582	2020.624	4314.605	418.477	3577.345	-40.621
4700	1113.914	2982.530	2040.836	4425.961	412.049	3646.025	-40.520
4800	1114.591	3005.989	2060.700	4537.386	405.271	3714.962	-40.426
4900	1115.227	3028.978	2080.227	4648.878	398.062	3783.895	-40.336
5000	1115.828	3051.514	2099.428	4760.431	390.525	3853.183	-40.253

3.426. Naphtho[7,8,1,2,3-*tu*vw]hexaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 119123-36-3
Point Group: C_s

Length: 17.96 Å
Width: 10.35 Å
Breadth: 3.885 Å
L/B Ratio: 1.734

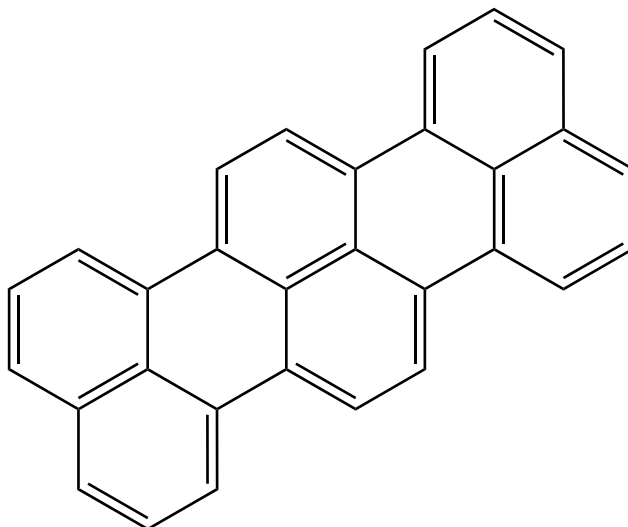
Cartesian coordinates:

C	6.3752	-1.5641	0.0000	C	-2.3971	-0.6326	0.0000	H	6.3197	1.8504	0.0000
C	6.8465	-0.2289	0.0000	C	-1.4919	-1.7048	0.0000	H	4.6495	-2.8538	0.0000
C	5.9635	0.8139	0.0000	C	1.7929	0.0777	0.0000	H	4.0315	2.6781	0.0000
C	5.0332	-1.8221	0.0000	C	0.3794	-0.1540	0.0000	H	1.7348	3.5316	0.0000
C	4.0871	-0.7591	0.0000	C	-0.1194	-1.4835	0.0000	H	-0.5584	4.3939	0.0000
C	4.5591	0.5730	0.0000	C	0.8203	-2.5730	0.0000	H	-2.9976	3.9802	0.0000
C	3.6457	1.6510	0.0000	C	2.1540	-2.3407	0.0000	H	-4.8814	2.4193	0.0000
C	2.2828	1.4198	0.0000	C	2.6828	-1.0036	0.0000	H	-1.8905	-2.7322	0.0000
C	1.3406	2.5077	0.0000	C	-3.8263	-0.8555	0.0000	H	0.4260	-3.5956	0.0000
C	-0.0025	2.2797	0.0000	C	-4.6997	0.2474	0.0000	H	2.8793	-3.1692	0.0000
C	-0.9583	3.3732	0.0000	C	-6.0961	0.0297	0.0000	H	-6.7709	0.8934	0.0000
C	-2.2838	3.1480	0.0000	C	-6.6007	-1.2500	0.0000	H	-7.6826	-1.4181	0.0000
C	-2.8280	1.8015	0.0000	C	-5.7298	-2.3529	0.0000	H	-6.1435	-3.3666	0.0000
C	-4.1751	1.5797	0.0000	C	-4.3679	-2.1592	0.0000	H	-3.6735	-3.0133	0.0000
C	-0.5178	0.9282	0.0000	H	7.1001	-2.3847	0.0000				
C	-1.9080	0.6914	0.0000	H	7.9260	-0.0460	0.0000				

Table 3.426: Table of thermodynamic data as a function of temperature for Naphtho[7,8,1,2,3-tuvwx]hexaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-54.149	478.123	478.123	∞
100	116.046	361.572	832.329	-47.076	504.521	551.802	-288.226
200	235.774	476.796	625.637	-29.768	490.497	604.689	-157.925
250	304.498	536.745	601.831	-16.272	483.946	633.994	-132.463
298.15	371.173	596.095	596.095	0.000	478.123	663.437	-116.229
300	373.700	598.399	596.102	0.689	477.908	664.585	-115.712
350	440.114	661.044	600.898	21.051	472.548	696.134	-103.890
400	501.682	723.893	612.346	44.619	467.900	728.390	-95.116
450	557.468	786.262	628.212	71.123	463.876	761.198	-88.356
500	607.348	847.630	647.096	100.267	460.384	794.447	-82.994
600	690.987	966.059	690.475	165.351	454.696	861.824	-75.027
700	757.058	1077.732	737.904	237.879	450.531	930.035	-69.399
800	809.934	1182.401	786.997	316.324	447.721	998.731	-65.209
900	852.911	1280.363	836.433	399.537	446.093	1067.700	-61.966
1000	888.317	1372.117	885.463	486.654	445.487	1136.808	-59.380
1100	917.805	1458.208	933.658	577.004	445.705	1205.946	-57.264
1200	942.585	1539.160	980.778	670.059	446.606	1275.014	-55.499
1300	963.564	1615.458	1026.693	765.395	448.004	1343.997	-54.001
1400	981.444	1687.538	1071.346	862.668	449.765	1412.862	-52.713
1500	996.774	1755.786	1114.721	961.598	451.812	1481.594	-51.593
1600	1009.990	1820.549	1156.829	1061.953	454.008	1550.173	-50.607
1700	1021.445	1882.131	1197.697	1163.538	456.281	1618.586	-49.732
1800	1031.424	1940.804	1237.364	1266.193	458.554	1686.935	-48.953
1900	1040.156	1996.809	1275.872	1369.781	460.796	1755.100	-48.250
2000	1047.834	2050.362	1313.268	1474.189	462.954	1823.178	-47.616
2100	1054.613	2101.653	1349.597	1579.318	464.945	1891.136	-47.038
2200	1060.623	2150.855	1384.907	1685.086	466.771	1959.006	-46.512
2300	1065.972	2198.122	1419.244	1791.421	468.428	2026.797	-46.029
2400	1070.751	2243.592	1452.650	1898.261	469.840	2094.467	-45.584
2500	1075.035	2287.391	1485.169	2005.554	471.023	2162.206	-45.176
2600	1078.888	2329.631	1516.841	2113.254	471.939	2229.775	-44.796
2700	1082.366	2370.415	1547.704	2221.319	472.593	2297.396	-44.445
2800	1085.513	2409.836	1577.794	2329.716	472.957	2365.018	-44.119
2900	1088.370	2447.979	1607.147	2438.412	473.001	2432.576	-43.815
3000	1090.970	2484.920	1635.793	2547.381	472.774	2500.167	-43.531
3100	1093.343	2520.732	1663.765	2656.599	472.192	2567.685	-43.264
3200	1095.513	2555.479	1691.091	2766.043	471.300	2635.308	-43.016
3300	1097.504	2589.221	1717.798	2875.695	470.080	2703.009	-42.784
3400	1099.333	2622.012	1743.913	2985.538	468.502	2770.654	-42.565
3500	1101.018	2653.904	1769.459	3095.557	466.570	2838.331	-42.359
3600	1102.573	2684.943	1794.460	3205.738	464.311	2906.167	-42.167
3700	1104.011	2715.172	1818.937	3316.068	461.689	2974.085	-41.986
3800	1105.343	2744.632	1842.912	3426.536	458.677	3042.017	-41.815
3900	1106.579	2773.360	1866.403	3537.133	455.320	3109.973	-41.653
4000	1107.728	2801.391	1889.428	3647.849	451.600	3178.174	-41.502
4100	1108.799	2828.757	1912.006	3758.676	447.479	3246.391	-41.359
4200	1109.797	2855.488	1934.153	3869.606	442.988	3314.703	-41.224
4300	1110.729	2881.613	1955.885	3980.633	438.110	3383.029	-41.095
4400	1111.601	2907.158	1977.215	4091.750	432.857	3451.572	-40.975
4500	1112.419	2932.149	1998.159	4202.952	427.245	3520.299	-40.862
4600	1113.185	2956.607	2018.730	4314.232	421.215	3589.167	-40.755
4700	1113.905	2980.555	2038.941	4425.587	414.786	3658.045	-40.654
4800	1114.582	3004.014	2058.803	4537.012	408.007	3727.180	-40.559
4900	1115.219	3027.002	2078.328	4648.502	400.797	3796.310	-40.468
5000	1115.819	3049.539	2097.528	4760.054	393.259	3865.796	-40.385

3.427. Tribenzo[*de,kl,rst*]pentaphene



Other names: Terrylene
Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 188-72-7
Point Group: D_{2h}

Length: 15.96 Å
Width: 9.168 Å
Breadth: 3.884 Å
L/B Ratio: 1.741

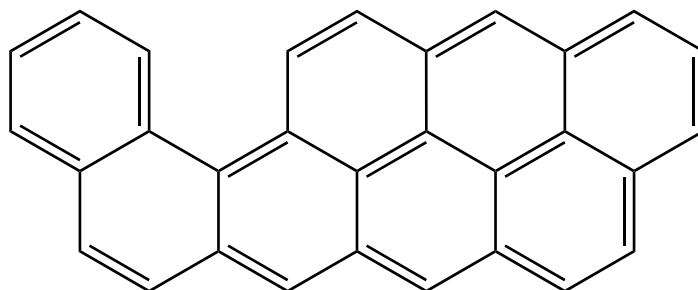
Cartesian coordinates:

C	2.8714	-1.2450	0.0000	C	-0.6993	2.4253	0.0000	H	6.7797	-1.2268	0.0000
C	3.5855	-2.4261	0.0000	C	-0.7073	0.0005	0.0000	H	6.7814	1.2172	0.0000
C	4.9943	-2.4217	0.0000	C	-1.4105	1.2415	0.0000	H	5.5333	3.3697	0.0000
C	5.6839	-1.2385	0.0000	C	-1.4123	-1.2395	0.0000	H	3.0491	3.3806	0.0000
C	2.8731	1.2409	0.0000	C	-2.8732	-1.2409	0.0000	H	-1.2477	-3.3812	0.0000
C	3.5717	-0.0025	0.0000	C	-5.6857	-1.2304	0.0000	H	1.2429	-3.3829	0.0000
C	4.9831	-0.0035	0.0000	C	-4.9978	-2.4146	0.0000	H	1.2478	3.3811	0.0000
C	5.6856	1.2305	0.0000	C	-3.5890	-2.4210	0.0000	H	-1.2429	3.3829	0.0000
C	4.9977	2.4146	0.0000	C	-3.5717	0.0025	0.0000	H	-6.7814	-1.2171	0.0000
C	3.5889	2.4210	0.0000	C	-2.8714	1.2450	0.0000	H	-5.5335	-3.3696	0.0000
C	1.4105	-1.2415	0.0000	C	-3.5855	2.4262	0.0000	H	-3.0492	-3.3806	0.0000
C	-0.7027	-2.4244	0.0000	C	-4.9943	2.4218	0.0000	H	-3.0443	3.3849	0.0000
C	0.6993	-2.4254	0.0000	C	-5.6839	1.2386	0.0000	H	-5.5286	3.3775	0.0000
C	0.7073	-0.0005	0.0000	C	-4.9831	0.0036	0.0000	H	-6.7797	1.2269	0.0000
C	1.4122	1.2395	0.0000	H	3.0444	-3.3849	0.0000				
C	0.7027	2.4243	0.0000	H	5.5287	-3.3775	0.0000				

Table 3.427: Table of thermodynamic data as a function of temperature for Tribenzo[*de,kl,rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-54.044	500.349	500.349	∞
100	116.278	355.991	824.110	-46.812	527.011	574.850	-300.265
200	234.259	470.790	618.670	-29.576	512.915	628.309	-164.094
250	302.485	530.341	595.017	-16.169	506.274	657.924	-137.463
298.15	368.960	589.316	589.316	0.000	500.349	687.684	-120.477
300	371.485	591.606	589.323	0.685	500.130	688.845	-119.936
350	437.918	653.909	594.092	20.936	494.659	720.742	-107.563
400	499.626	716.473	605.480	44.397	489.905	753.362	-98.377
450	555.601	778.611	621.272	70.803	485.782	786.547	-91.298
500	605.672	839.792	640.074	99.859	482.202	820.184	-85.682
600	689.636	957.946	683.293	164.792	476.363	888.359	-77.337
700	755.936	1069.429	730.575	237.198	472.075	957.391	-71.440
800	808.968	1173.959	779.537	315.538	469.161	1026.925	-67.050
900	852.055	1271.814	828.858	398.661	467.442	1096.744	-63.652
1000	887.543	1363.482	877.786	485.696	466.756	1166.711	-60.941
1100	917.099	1449.502	925.891	575.972	466.900	1236.717	-58.726
1200	941.936	1530.396	972.930	668.959	467.732	1306.658	-56.876
1300	962.967	1606.644	1018.773	764.233	469.068	1376.520	-55.308
1400	980.892	1678.681	1063.360	861.449	470.772	1446.269	-53.960
1500	996.263	1746.893	1106.675	960.326	472.766	1515.888	-52.787
1600	1009.517	1811.624	1148.729	1060.631	474.913	1585.358	-51.756
1700	1021.007	1873.178	1189.548	1162.171	477.140	1654.665	-50.841
1800	1031.017	1931.827	1229.170	1264.783	479.371	1723.910	-50.026
1900	1039.778	1987.811	1267.636	1368.333	481.574	1792.975	-49.291
2000	1047.482	2041.345	1304.993	1472.704	483.695	1861.953	-48.628
2100	1054.285	2092.620	1341.287	1577.799	485.653	1930.814	-48.025
2200	1060.317	2141.807	1376.564	1683.535	487.447	1999.588	-47.475
2300	1065.686	2189.061	1410.869	1789.841	489.074	2068.284	-46.971
2400	1070.483	2234.519	1444.247	1896.653	490.459	2136.861	-46.507
2500	1074.784	2278.307	1476.739	2003.921	491.616	2205.508	-46.081
2600	1078.653	2320.538	1508.385	2111.596	492.507	2273.986	-45.684
2700	1082.144	2361.313	1539.225	2219.639	493.138	2342.517	-45.318
2800	1085.305	2400.726	1569.293	2328.014	493.481	2411.050	-44.978
2900	1088.173	2438.862	1598.624	2436.690	493.505	2479.519	-44.660
3000	1090.785	2475.797	1627.251	2545.640	493.259	2548.022	-44.364
3100	1093.167	2511.603	1655.203	2654.839	492.659	2616.452	-44.086
3200	1095.347	2546.345	1682.511	2764.267	491.750	2684.989	-43.827
3300	1097.347	2580.081	1709.202	2873.903	490.514	2753.603	-43.585
3400	1099.184	2612.868	1735.300	2983.731	488.920	2822.162	-43.356
3500	1100.876	2644.756	1760.831	3093.735	486.974	2890.754	-43.141
3600	1102.438	2675.790	1785.818	3203.901	484.701	2959.505	-42.940
3700	1103.882	2706.016	1810.281	3314.218	482.066	3028.339	-42.752
3800	1105.220	2735.473	1834.243	3424.674	479.042	3097.186	-42.573
3900	1106.462	2764.198	1857.721	3535.259	475.673	3166.058	-42.404
4000	1107.617	2792.225	1880.734	3645.964	471.941	3235.175	-42.246
4100	1108.692	2819.589	1903.301	3756.780	467.809	3304.309	-42.097
4200	1109.695	2846.318	1925.437	3867.700	463.307	3373.539	-41.955
4300	1110.632	2872.441	1947.158	3978.717	458.420	3442.781	-41.821
4400	1111.508	2897.984	1968.478	4089.824	453.158	3512.242	-41.695
4500	1112.329	2922.972	1989.412	4201.017	447.536	3581.887	-41.577
4600	1113.099	2947.428	2009.974	4312.288	441.498	3651.673	-41.465
4700	1113.822	2971.374	2030.175	4423.635	435.060	3721.468	-41.359
4800	1114.502	2994.831	2050.029	4535.051	428.273	3791.521	-41.259
4900	1115.143	3017.818	2069.546	4646.534	421.055	3861.570	-41.164
5000	1115.746	3040.353	2088.737	4758.079	413.510	3931.974	-41.076

3.428. Anthra[8,9,1,2-*lmnop*]benzo[*a*]naphthacene



Formula: $C_{30}H_{16}$
Mass: 376.448 g/mol
CAS Number: 120835-87-2
Point Group: C_1

Length: 16.82 Å
Width: 9.515 Å
Breadth: 4.901 Å
L/B Ratio: 1.767

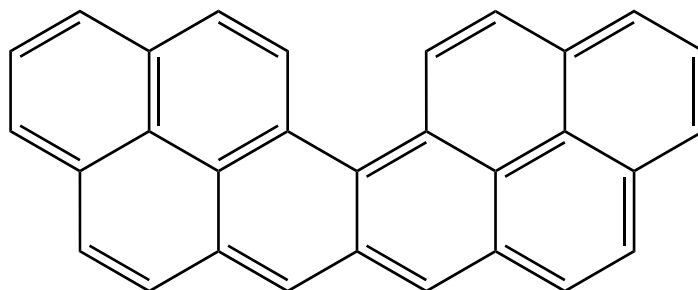
Cartesian coordinates:

C	6.3477	-1.5858	-0.4032	C	-4.8444	0.5430	-0.1877	H	3.0495	-2.2874	-0.8208
C	6.2541	-0.2659	-0.0198	C	-6.0616	-0.1133	-0.2107	H	5.2551	-3.3329	-1.0566
C	3.9443	-1.7066	-0.5588	C	-6.1162	-1.5121	-0.0822	H	5.8800	2.3067	0.5336
C	5.1811	-2.2994	-0.7023	C	-4.9671	-2.2507	0.0703	H	3.7071	3.5067	0.4468
C	3.8089	-0.3779	-0.1046	C	-2.3827	0.4534	-0.0143	H	1.3688	3.5247	0.1249
C	4.9958	0.3567	0.0981	C	-3.6426	-0.2061	-0.0341	H	-1.0508	3.6130	-0.1843
C	4.9406	1.7709	0.3551	C	-3.7041	-1.6112	0.0988	H	-3.5029	3.7061	-0.3856
C	3.7586	2.4187	0.3212	C	-2.5033	-2.3488	0.2644	H	-5.6898	2.5420	-0.4320
C	2.5190	0.2777	0.0792	C	0.0698	0.3630	0.1174	H	-6.9914	0.4545	-0.3291
C	2.5220	1.6967	0.1517	C	-1.2043	-0.2894	0.1278	H	-7.0912	-2.0104	-0.1041
C	1.3351	2.4279	0.1034	C	-1.2838	-1.7089	0.2833	H	-5.0139	-3.3408	0.1718
C	0.1031	1.7781	0.0280	C	-0.0507	-2.4292	0.4856	H	-2.5602	-3.4380	0.3810
C	-1.1112	2.5205	-0.1056	C	1.1426	-1.8011	0.4452	H	-0.1136	-3.5044	0.6904
C	-2.3225	1.8847	-0.1388	C	1.2726	-0.3830	0.1923	H	2.0571	-2.3791	0.6379
C	-3.5650	2.6158	-0.2905	H	7.3244	-2.0716	-0.4942				
C	-4.7540	1.9831	-0.3154	H	7.1604	0.3172	0.1808				

Table 3.428: Table of thermodynamic data as a function of temperature for Anthra[8,9,1,2-*lmnop*]benzo[*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.443	499.057	499.057	∞
100	112.687	355.885	822.101	-46.622	525.909	573.758	-299.694
200	233.574	469.101	617.086	-29.597	511.602	627.333	-163.839
250	302.786	528.614	593.404	-16.197	504.953	657.035	-137.277
298.15	369.783	587.692	587.692	0.000	499.057	686.876	-120.335
300	372.321	589.987	587.699	0.686	498.839	688.039	-119.796
350	438.972	652.439	592.479	20.986	493.417	720.014	-107.454
400	500.717	715.148	603.895	44.501	488.716	752.704	-98.291
450	556.643	777.411	619.722	70.960	484.647	785.952	-91.229
500	606.635	838.698	638.565	100.066	481.117	819.646	-85.626
600	690.439	957.013	681.868	165.087	475.366	887.922	-77.299
700	756.623	1068.611	729.229	237.567	471.152	957.041	-71.414
800	809.580	1173.227	778.262	315.972	468.303	1026.653	-67.032
900	852.615	1271.151	827.647	399.154	466.643	1096.541	-63.640
1000	888.066	1362.876	876.633	486.243	466.010	1166.572	-60.934
1100	917.589	1448.944	924.790	576.570	466.205	1236.636	-58.722
1200	942.396	1529.879	971.876	669.604	467.085	1306.630	-56.875
1300	963.399	1606.163	1017.761	764.922	468.465	1376.542	-55.309
1400	981.297	1678.231	1062.388	862.181	470.211	1446.338	-53.962
1500	996.642	1746.470	1105.739	961.097	472.244	1516.001	-52.791
1600	1009.872	1811.225	1147.825	1061.439	474.427	1585.511	-51.761
1700	1021.339	1872.800	1188.675	1163.013	476.689	1654.858	-50.847
1800	1031.327	1931.467	1228.324	1265.657	478.952	1724.140	-50.032
1900	1040.068	1987.467	1266.817	1369.236	481.185	1793.239	-49.299
2000	1047.753	2041.016	1304.198	1473.636	483.334	1862.251	-48.636
2100	1054.539	2092.303	1340.514	1578.757	485.318	1931.145	-48.034
2200	1060.555	2141.502	1375.812	1684.518	487.137	1999.949	-47.484
2300	1065.909	2188.766	1410.137	1790.846	488.787	2068.676	-46.980
2400	1070.692	2234.234	1443.533	1897.681	490.193	2137.281	-46.516
2500	1074.981	2278.030	1476.043	2004.968	491.371	2205.956	-46.090
2600	1078.838	2320.268	1507.705	2112.662	492.281	2274.462	-45.694
2700	1082.319	2361.050	1538.560	2220.723	492.930	2343.019	-45.327
2800	1085.469	2400.469	1568.642	2329.115	493.290	2411.578	-44.988
2900	1088.328	2438.610	1597.987	2437.807	493.330	2480.073	-44.670
3000	1090.931	2475.551	1626.627	2546.772	493.099	2548.600	-44.374
3100	1093.306	2511.362	1654.592	2655.986	492.513	2617.055	-44.096
3200	1095.479	2546.107	1681.912	2765.427	491.618	2685.616	-43.837
3300	1097.471	2579.848	1708.613	2875.076	490.394	2754.253	-43.595
3400	1099.302	2612.638	1734.722	2984.916	488.812	2822.836	-43.367
3500	1100.989	2644.529	1760.263	3094.931	486.878	2891.451	-43.152
3600	1102.545	2675.567	1785.259	3205.109	484.616	2960.224	-42.951
3700	1103.984	2705.796	1809.732	3315.436	481.991	3029.080	-42.762
3800	1105.318	2735.255	1833.702	3425.902	478.977	3097.949	-42.583
3900	1106.555	2763.982	1857.188	3536.497	475.618	3166.843	-42.414
4000	1107.706	2792.012	1880.210	3647.210	471.895	3235.982	-42.257
4100	1108.777	2819.378	1902.784	3758.035	467.772	3305.136	-42.107
4200	1109.776	2846.109	1924.927	3868.963	463.278	3374.387	-41.966
4300	1110.710	2872.234	1946.655	3979.988	458.399	3443.650	-41.831
4400	1111.583	2897.778	1967.982	4091.103	453.144	3513.132	-41.705
4500	1112.401	2922.768	1988.923	4202.303	447.530	3582.797	-41.587
4600	1113.168	2947.226	2009.491	4313.582	441.499	3652.603	-41.476
4700	1113.888	2971.174	2029.698	4424.935	435.068	3722.419	-41.369
4800	1114.566	2994.632	2049.557	4536.358	428.287	3792.492	-41.270
4900	1115.204	3017.620	2069.080	4647.847	421.076	3862.561	-41.175
5000	1115.805	3040.156	2088.277	4759.398	413.536	3932.984	-41.087

3.429. Dinaphtho[8,1,2-*lmn*:2',1',8'-*gra*]naphthacene



Formula: $C_{30}H_{16}$
Mass: 376.448 g/mol
CAS Number: 58052-99-6
Point Group: C_2

Length: 16.80 Å
Width: 9.445 Å
Breadth: 4.950 Å
L/B Ratio: 1.779

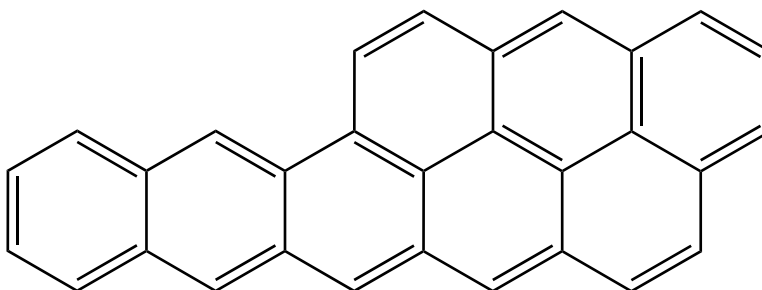
Cartesian coordinates:

C	-4.8416	1.8938	0.4081	C	2.6087	-2.3644	0.5696	H	-1.1650	3.5389	0.1861
C	-3.6496	2.5220	0.4073	C	1.4037	-1.7455	0.4907	H	1.1650	3.5389	-0.1861
C	-2.4168	1.7942	0.1961	C	1.2717	-0.3617	0.1324	H	3.5793	3.6037	-0.5711
C	-1.2093	2.4439	0.1273	C	2.4578	0.3767	-0.0163	H	5.7741	2.4440	-0.5780
C	0.0000	0.2972	0.0000	C	-4.9301	0.4699	0.1742	H	7.0808	0.3867	-0.3140
C	0.0000	1.7129	0.0000	C	-5.0743	-2.2832	-0.3342	H	7.2009	-2.0506	0.1235
C	1.2093	2.4439	-0.1272	C	-6.2251	-1.5538	-0.1058	H	5.1295	-3.3580	0.5401
C	2.4168	1.7941	-0.1961	C	-6.1584	-0.1802	0.1437	H	2.6791	-3.4222	0.8484
C	3.6496	2.5220	-0.4073	C	-3.8194	-1.6495	-0.3058	H	0.4965	-2.3167	0.7307
C	4.8415	1.8938	-0.4081	C	-3.7372	-0.2687	-0.0368	H	-5.1295	-3.3580	-0.5401
C	4.9301	0.4699	-0.1743	C	-2.4578	0.3767	0.0163	H	-7.2008	-2.0507	-0.1235
C	6.1584	-0.1802	-0.1437	C	-1.2718	-0.3616	-0.1323	H	-7.0808	0.3867	0.3140
C	6.2251	-1.5537	0.1057	C	-1.4037	-1.7454	-0.4906	H	-0.4967	-2.3169	-0.7307
C	5.0743	-2.2832	0.3342	C	-2.6086	-2.3644	-0.5696	H	-2.6793	-3.4222	-0.8484
C	3.7372	-0.2687	0.0368	H	-5.7741	2.4440	0.5780				
C	3.8195	-1.6495	0.3057	H	-3.5794	3.6037	0.5711				

Table 3.429: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*lmn*:2',1',8'-*qra*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.173	488.178	488.178	∞
100	111.428	348.677	812.961	-46.428	515.224	563.794	-294.490
200	232.632	461.069	608.672	-29.521	500.800	618.137	-161.438
250	302.026	520.394	585.046	-16.163	494.109	648.246	-135.441
298.15	369.110	579.346	579.346	0.000	488.178	678.486	-118.865
300	371.650	581.637	579.353	0.685	487.960	679.665	-118.338
350	438.343	643.989	584.125	20.952	482.505	712.060	-106.267
400	500.116	706.615	595.523	44.437	477.773	745.174	-97.308
450	556.068	768.810	611.329	70.866	473.675	778.851	-90.405
500	606.088	830.037	630.148	99.945	470.117	812.976	-84.929
600	689.954	948.258	673.402	164.914	464.314	882.123	-76.794
700	756.199	1059.785	720.716	237.348	460.055	952.122	-71.047
800	809.212	1164.349	769.707	315.714	457.166	1022.618	-66.769
900	852.296	1262.232	819.053	398.861	455.471	1093.397	-63.458
1000	887.787	1353.926	868.005	485.921	454.809	1164.321	-60.817
1100	917.344	1439.969	916.132	576.221	454.977	1235.281	-58.657
1200	942.181	1520.884	963.190	669.232	455.835	1306.174	-56.855
1300	963.208	1597.152	1009.052	764.530	457.195	1376.987	-55.327
1400	981.127	1669.206	1053.656	861.771	458.923	1447.684	-54.013
1500	996.490	1737.434	1096.987	960.671	460.939	1518.250	-52.869
1600	1009.735	1802.180	1139.056	1060.998	463.109	1588.665	-51.864
1700	1021.215	1863.747	1179.889	1162.559	465.358	1658.916	-50.971
1800	1031.215	1922.407	1219.523	1265.192	467.608	1729.103	-50.176
1900	1039.966	1978.402	1258.002	1368.760	469.831	1799.109	-49.460
2000	1047.660	2031.945	1295.370	1473.150	471.970	1869.028	-48.813
2100	1054.453	2083.228	1331.675	1578.262	473.945	1938.829	-48.225
2200	1060.476	2132.423	1366.962	1684.015	475.755	2008.541	-47.688
2300	1065.836	2179.684	1401.277	1790.335	477.398	2078.175	-47.196
2400	1070.625	2225.148	1434.664	1897.163	478.797	2147.689	-46.742
2500	1074.918	2268.942	1467.165	2004.444	479.968	2217.273	-46.326
2600	1078.780	2311.178	1498.819	2112.132	480.873	2286.688	-45.939
2700	1082.264	2351.958	1529.666	2220.187	481.516	2356.154	-45.582
2800	1085.418	2391.375	1559.741	2328.574	481.871	2425.622	-45.250
2900	1088.281	2429.514	1589.080	2437.261	481.906	2495.026	-44.939
3000	1090.886	2466.454	1617.713	2546.222	481.670	2564.464	-44.650
3100	1093.264	2502.263	1645.672	2655.431	481.079	2633.828	-44.379
3200	1095.439	2537.007	1672.986	2764.868	480.180	2703.299	-44.126
3300	1097.434	2570.747	1699.682	2874.513	478.953	2772.846	-43.890
3400	1099.267	2603.536	1725.786	2984.349	477.368	2842.339	-43.666
3500	1100.955	2635.426	1751.323	3094.361	475.430	2911.864	-43.456
3600	1102.514	2666.463	1776.314	3204.536	473.164	2981.548	-43.260
3700	1103.955	2696.691	1800.782	3314.860	470.537	3051.314	-43.076
3800	1105.289	2726.149	1824.748	3425.323	467.520	3121.094	-42.902
3900	1106.528	2754.876	1848.231	3535.915	464.157	3190.898	-42.736
4000	1107.680	2782.905	1871.249	3646.626	460.433	3260.948	-42.583
4100	1108.753	2810.270	1893.819	3757.448	456.307	3331.013	-42.437
4200	1109.753	2837.000	1915.959	3868.374	451.811	3401.175	-42.299
4300	1110.687	2863.125	1937.683	3979.397	446.929	3471.349	-42.168
4400	1111.561	2888.669	1959.008	4090.510	441.672	3541.741	-42.045
4500	1112.380	2913.658	1979.945	4201.707	436.056	3612.317	-41.930
4600	1113.148	2938.115	2000.510	4312.984	430.022	3683.035	-41.821
4700	1113.869	2962.063	2020.715	4424.335	423.590	3753.761	-41.718
4800	1114.548	2985.521	2040.572	4535.756	416.807	3824.746	-41.621
4900	1115.186	3008.509	2060.092	4647.243	409.594	3895.725	-41.528
5000	1115.788	3031.044	2079.286	4758.792	402.053	3967.060	-41.443

3.430. Anthra[2,1,9,8-*stuv*a]pentacene



Formula: $C_{30}H_{16}$
Mass: 376.448 g/mol
CAS Number: 120835-88-3
Point Group: C_s

Length: 17.76 Å
Width: 9.579 Å
Breadth: 3.886 Å
L/B Ratio: 1.854

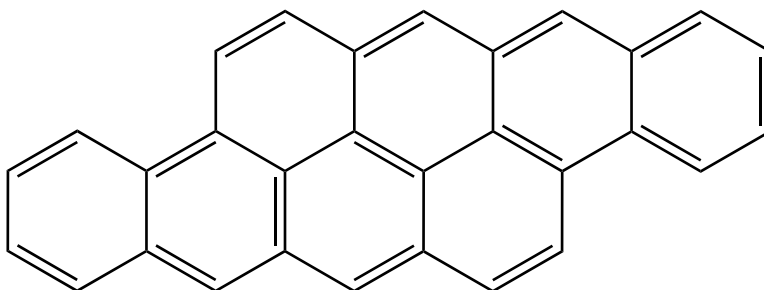
Cartesian coordinates:

C	7.1169	-1.0153	0.0000	C	-4.9702	0.8590	0.0000	H	6.4137	2.3358	0.0000
C	7.3230	0.3968	0.0000	C	-6.2549	0.3590	0.0000	H	5.6914	-2.6136	0.0000
C	6.2656	1.2499	0.0000	C	-6.4774	-1.0344	0.0000	H	3.9808	2.6872	0.0000
C	5.8598	-1.5308	0.0000	C	-5.4271	-1.9141	0.0000	H	3.2515	-2.2601	0.0000
C	4.7168	-0.6635	0.0000	C	-2.5348	0.4574	0.0000	H	1.5803	3.0537	0.0000
C	4.9220	0.7454	0.0000	C	-3.8602	-0.0402	0.0000	H	-0.8338	3.4480	0.0000
C	3.8245	1.6012	0.0000	C	-4.0880	-1.4365	0.0000	H	-3.2575	3.8459	0.0000
C	3.4205	-1.1712	0.0000	C	-2.9893	-2.3228	0.0000	H	-5.5693	2.9597	0.0000
C	2.3094	-0.3168	0.0000	C	-0.1090	0.0637	0.0000	H	-7.1136	1.0397	0.0000
C	2.5165	1.0914	0.0000	C	-1.4540	-0.4322	0.0000	H	-7.5080	-1.4050	0.0000
C	1.3997	1.9715	0.0000	C	-1.6918	-1.8390	0.0000	H	-5.6025	-2.9958	0.0000
C	0.1133	1.4818	0.0000	C	-0.5559	-2.7244	0.0000	H	-3.1740	-3.4041	0.0000
C	-1.0222	2.3672	0.0000	C	0.7068	-2.2373	0.0000	H	-0.7436	-3.8043	0.0000
C	-2.2960	1.8834	0.0000	C	0.9669	-0.8231	0.0000	H	1.5781	-2.9105	0.0000
C	-3.4485	2.7663	0.0000	H	7.9928	-1.6724	0.0000				
C	-4.7054	2.2849	0.0000	H	8.3501	0.7762	0.0000				

Table 3.430: Table of thermodynamic data as a function of temperature for Anthra[2,1,9,8-*stuv*a]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-53.892	498.482	498.482	∞
100	114.465	360.519	829.616	-46.910	525.047	572.432	-299.002
200	234.990	474.852	623.482	-29.726	510.898	625.479	-163.355
250	304.098	534.669	599.703	-16.258	504.318	654.886	-136.828
298.15	371.006	593.971	593.971	0.000	498.482	684.429	-119.907
300	373.540	596.273	593.978	0.689	498.267	685.581	-119.368
350	440.090	658.906	598.772	21.047	492.903	717.237	-107.040
400	501.731	721.757	610.219	44.615	488.256	749.600	-97.886
450	557.558	784.134	626.084	71.122	484.235	782.515	-90.830
500	607.461	845.513	644.968	100.272	480.749	815.870	-85.232
600	691.126	963.965	688.351	165.368	475.073	883.457	-76.910
700	757.213	1075.661	735.787	237.912	470.922	951.876	-71.028
800	810.102	1180.351	784.886	316.372	468.129	1020.779	-66.649
900	853.087	1278.334	834.330	399.603	466.518	1089.952	-63.258
1000	888.496	1370.106	883.369	486.738	465.930	1159.262	-60.552
1100	917.985	1456.214	931.572	577.106	466.166	1228.600	-58.340
1200	942.762	1537.182	978.700	670.178	467.084	1297.866	-56.493
1300	963.736	1613.494	1024.624	765.531	468.500	1367.047	-54.927
1400	981.609	1685.586	1069.284	862.822	470.278	1436.108	-53.581
1500	996.931	1753.846	1112.667	961.768	472.341	1505.034	-52.409
1600	1010.140	1818.618	1154.782	1062.138	474.552	1573.806	-51.378
1700	1021.587	1880.209	1195.658	1163.738	476.840	1642.413	-50.464
1800	1031.557	1938.890	1235.331	1266.406	479.126	1710.953	-49.650
1900	1040.282	1994.902	1273.846	1370.007	481.382	1779.309	-48.916
2000	1047.952	2048.461	1311.247	1474.427	483.552	1847.578	-48.253
2100	1054.724	2099.758	1347.583	1579.568	485.554	1915.726	-47.650
2200	1060.727	2148.965	1382.898	1685.346	487.391	1983.785	-47.100
2300	1066.070	2196.236	1417.240	1791.691	489.058	2051.764	-46.596
2400	1070.843	2241.711	1450.652	1898.541	490.480	2119.622	-46.131
2500	1075.122	2285.513	1483.175	2005.844	491.672	2187.550	-45.705
2600	1078.970	2327.756	1514.852	2113.551	492.596	2255.307	-45.309
2700	1082.443	2368.543	1545.719	2221.625	493.258	2323.115	-44.942
2800	1085.586	2407.967	1575.814	2330.029	493.630	2390.924	-44.602
2900	1088.439	2446.112	1605.170	2438.733	493.681	2458.669	-44.284
3000	1091.035	2483.056	1633.820	2547.708	493.461	2526.446	-43.988
3100	1093.405	2518.870	1661.795	2656.932	492.885	2594.151	-43.710
3200	1095.572	2553.619	1689.125	2766.383	491.999	2661.960	-43.451
3300	1097.560	2587.363	1715.835	2876.041	490.785	2729.846	-43.209
3400	1099.386	2620.155	1741.953	2985.889	489.212	2797.677	-42.980
3500	1101.068	2652.049	1767.502	3095.913	487.285	2865.540	-42.765
3600	1102.621	2683.089	1792.506	3206.098	485.031	2933.561	-42.564
3700	1104.056	2713.319	1816.986	3316.433	482.414	3001.665	-42.375
3800	1105.386	2742.780	1840.963	3426.906	479.407	3069.782	-42.196
3900	1106.621	2771.509	1864.456	3537.507	476.054	3137.923	-42.027
4000	1107.768	2799.541	1887.484	3648.228	472.338	3206.309	-41.869
4100	1108.837	2826.908	1910.065	3759.058	468.221	3274.711	-41.719
4200	1109.833	2853.641	1932.214	3869.992	463.733	3343.208	-41.578
4300	1110.764	2879.767	1953.947	3981.023	458.859	3411.718	-41.443
4400	1111.635	2905.313	1975.280	4092.143	453.610	3480.446	-41.317
4500	1112.451	2930.303	1996.226	4203.348	448.000	3549.358	-41.199
4600	1113.216	2954.762	2016.799	4314.632	441.974	3618.410	-41.087
4700	1113.935	2978.711	2037.011	4425.990	435.548	3687.472	-40.981
4800	1114.610	3002.171	2056.875	4537.417	428.772	3756.792	-40.881
4900	1115.246	3025.160	2076.402	4648.910	421.565	3826.107	-40.786
5000	1115.846	3047.697	2095.604	4760.465	414.030	3895.776	-40.698

3.431. Naphthaceno[2,1,12,11-*opqra*]naphthacene



Formula: $C_{30}H_{16}$
Mass: 376.448 g/mol
CAS Number: 188-42-1
Point Group: C_{2h}

Length: 17.76 Å
Width: 9.554 Å
Breadth: 3.885 Å
L/B Ratio: 1.859

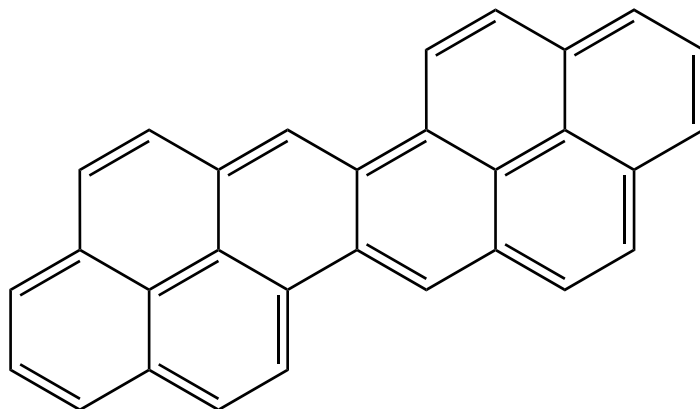
Cartesian coordinates:

C	6.6716	-0.8632	0.0000	C	-1.0433	-2.3188	0.0000	H	6.0581	2.4989	0.0000
C	6.9176	0.5364	0.0000	C	-0.5270	0.4573	0.0000	H	5.1868	-2.4197	0.0000
C	5.8788	1.4177	0.0000	C	0.5269	-0.4573	0.0000	H	3.6635	2.9352	0.0000
C	5.3948	-1.3387	0.0000	C	0.2515	-1.8683	0.0000	H	1.2583	3.3946	0.0000
C	4.2792	-0.4463	0.0000	C	1.3726	-2.7820	0.0000	H	-1.1563	3.8566	0.0000
C	4.5267	0.9503	0.0000	C	2.6432	-2.3291	0.0000	H	-3.4981	3.0230	0.0000
C	3.4576	1.8576	0.0000	C	2.9448	-0.9167	0.0000	H	-3.6634	-2.9353	0.0000
C	2.1406	1.4037	0.0000	C	1.8806	0.0026	0.0000	H	-1.2583	-3.3946	0.0000
C	1.0433	2.3188	0.0000	C	-4.5267	-0.9504	0.0000	H	1.1564	-3.8566	0.0000
C	-0.2515	1.8683	0.0000	C	-4.2792	0.4463	0.0000	H	3.4982	-3.0230	0.0000
C	-1.3726	2.7820	0.0000	C	-5.3948	1.3387	0.0000	H	-5.1867	2.4197	0.0000
C	-2.6432	2.3291	0.0000	C	-6.6716	0.8633	0.0000	H	-7.5240	1.5504	0.0000
C	-2.9449	0.9167	0.0000	C	-6.9176	-0.5364	0.0000	H	-7.9534	-0.8911	0.0000
C	-3.4576	-1.8576	0.0000	C	-5.8789	-1.4176	0.0000	H	-6.0581	-2.4989	0.0000
C	-1.8806	-0.0026	0.0000	H	7.5240	-1.5504	0.0000				
C	-2.1406	-1.4037	0.0000	H	7.9534	0.8912	0.0000				

Table 3.431: Table of thermodynamic data as a function of temperature for Naphthaceno[2,1,12,11-*opqra*]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-53.860	501.188	501.188	∞
100	115.081	352.841	821.720	-46.888	527.774	575.927	-300.827
200	234.848	467.406	615.783	-29.675	513.654	629.724	-164.464
250	303.555	527.147	592.048	-16.225	507.057	659.505	-137.793
298.15	370.192	586.328	586.328	0.000	501.188	689.414	-120.780
300	372.718	588.625	586.335	0.687	500.971	690.580	-120.238
350	439.105	651.117	591.118	21.000	495.561	722.621	-107.843
400	500.672	713.831	602.539	44.517	490.863	755.377	-98.640
450	556.482	776.082	618.371	70.970	486.788	788.691	-91.547
500	606.403	837.348	637.215	100.066	483.248	822.452	-85.919
600	690.147	955.614	680.513	165.060	477.470	890.866	-77.555
700	756.325	1067.166	727.865	237.511	473.227	960.127	-71.644
800	809.297	1171.743	776.885	315.886	470.348	1029.885	-67.243
900	852.356	1269.635	826.256	399.041	468.661	1099.923	-63.837
1000	887.829	1361.334	875.229	486.106	468.003	1170.107	-61.119
1100	917.375	1447.381	923.372	576.410	468.175	1240.326	-58.897
1200	942.204	1528.298	970.445	669.424	469.036	1310.478	-57.042
1300	963.225	1604.567	1016.318	764.724	470.397	1380.549	-55.470
1400	981.139	1676.623	1060.933	861.965	472.127	1450.505	-54.118
1500	996.499	1744.852	1104.274	960.866	474.144	1520.329	-52.941
1600	1009.742	1809.597	1146.351	1061.195	476.314	1590.002	-51.907
1700	1021.220	1871.165	1187.191	1162.756	478.564	1659.511	-50.990
1800	1031.218	1929.826	1226.832	1265.389	480.815	1728.957	-50.172
1900	1039.969	1985.821	1265.316	1368.958	483.038	1798.221	-49.436
2000	1047.662	2039.364	1302.690	1473.348	485.178	1867.398	-48.770
2100	1054.454	2090.647	1338.999	1578.461	487.152	1936.457	-48.166
2200	1060.477	2139.842	1374.291	1684.213	488.963	2005.427	-47.614
2300	1065.837	2187.103	1408.610	1790.534	490.606	2074.320	-47.108
2400	1070.625	2232.567	1442.000	1897.361	492.005	2143.092	-46.642
2500	1074.918	2276.361	1474.504	2004.642	493.176	2211.934	-46.215
2600	1078.780	2318.597	1506.162	2112.331	494.081	2280.607	-45.817
2700	1082.264	2359.377	1537.011	2220.386	494.724	2349.331	-45.450
2800	1085.418	2398.794	1567.089	2328.772	495.078	2418.057	-45.108
2900	1088.280	2436.933	1596.430	2437.460	495.114	2486.719	-44.790
3000	1090.886	2473.872	1625.066	2546.420	494.878	2555.415	-44.493
3100	1093.264	2509.682	1653.027	2655.629	494.287	2624.038	-44.214
3200	1095.439	2544.426	1680.343	2765.066	493.388	2692.766	-43.954
3300	1097.433	2578.166	1707.041	2874.711	492.161	2761.572	-43.711
3400	1099.267	2610.955	1733.147	2984.547	490.575	2830.323	-43.482
3500	1100.955	2642.845	1758.685	3094.559	488.637	2899.106	-43.266
3600	1102.513	2673.882	1783.678	3204.734	486.372	2968.048	-43.064
3700	1103.954	2704.109	1808.148	3315.058	483.744	3037.073	-42.875
3800	1105.289	2733.568	1832.115	3425.521	480.727	3106.110	-42.696
3900	1106.528	2762.294	1855.599	3536.113	477.365	3175.173	-42.526
4000	1107.679	2790.324	1878.618	3646.824	473.640	3244.480	-42.368
4100	1108.752	2817.689	1901.190	3757.646	469.514	3313.804	-42.218
4200	1109.752	2844.419	1923.331	3868.572	465.018	3383.224	-42.076
4300	1110.687	2870.543	1945.056	3979.594	460.136	3452.656	-41.941
4400	1111.561	2896.087	1966.381	4090.707	454.879	3522.306	-41.814
4500	1112.380	2921.077	1987.320	4201.904	449.262	3592.141	-41.696
4600	1113.148	2945.534	2007.886	4313.181	443.229	3662.116	-41.584
4700	1113.869	2969.481	2028.092	4424.532	436.796	3732.101	-41.477
4800	1114.547	2992.939	2047.949	4535.954	430.013	3802.343	-41.377
4900	1115.186	3015.927	2067.470	4647.441	422.800	3872.581	-41.281
5000	1115.788	3038.463	2086.665	4758.990	415.259	3943.174	-41.193

3.432. Benzo[*pqr*]naphtho[8,1,2-*cde*]picene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 111728-58-6
Point Group: C_{2h}

Length: 17.95 Å
Width: 9.550 Å
Breadth: 3.888 Å
L/B Ratio: 1.879

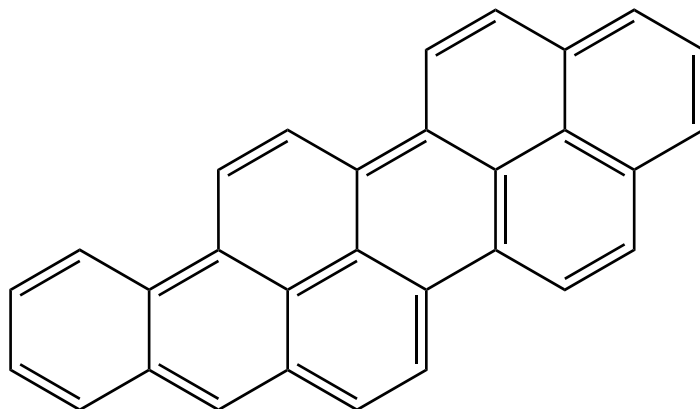
Cartesian coordinates:

C	4.3025	-2.4164	0.0000	C	-4.4604	-1.3400	0.0000	H	0.2684	-2.7713	0.0000
C	2.9711	-2.6306	0.0000	C	-3.5396	-2.4386	0.0000	H	-0.2686	2.7714	0.0000
C	2.0311	-1.5303	0.0000	C	-2.1998	-2.2219	0.0000	H	-2.5633	3.6480	0.0000
C	0.6721	-1.7460	0.0000	C	-1.6567	-0.8948	0.0000	H	-5.0103	3.2533	0.0000
C	-0.2431	-0.6632	0.0000	C	4.8454	-1.0760	0.0000	H	-6.9125	1.6925	0.0000
C	0.2430	0.6632	0.0000	C	6.2165	-0.8461	0.0000	H	-7.7949	-0.6245	0.0000
C	-0.6722	1.7460	0.0000	C	6.7121	0.4607	0.0000	H	-6.2466	-2.5648	0.0000
C	-2.0311	1.5303	0.0000	C	5.8518	1.5425	0.0000	H	-3.9448	-3.4569	0.0000
C	-2.9712	2.6306	0.0000	C	3.9519	0.0248	0.0000	H	-1.4900	-3.0633	0.0000
C	-4.3025	2.4163	0.0000	C	4.4604	1.3400	0.0000	H	6.9127	-1.6925	0.0000
C	-4.8453	1.0760	0.0000	C	3.5396	2.4387	0.0000	H	7.7950	0.6243	0.0000
C	-6.2165	0.8461	0.0000	C	2.1998	2.2219	0.0000	H	6.2466	2.5648	0.0000
C	-6.7120	-0.4607	0.0000	C	1.6566	0.8948	0.0000	H	3.9449	3.4570	0.0000
C	-5.8517	-1.5425	0.0000	C	2.5364	-0.1932	0.0000	H	1.4901	3.0634	0.0000
C	-2.5364	0.1932	0.0000	H	5.0103	-3.2534	0.0000				
C	-3.9519	-0.0248	0.0000	H	2.5632	-3.6481	0.0000				

Table 3.432: Table of thermodynamic data as a function of temperature for Benzo[*pqr*]naphtho[8,1,2-*cde*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.817	461.814	461.814	∞
100	114.365	357.062	825.036	-46.797	488.490	536.221	-280.088
200	234.376	471.107	619.398	-29.658	474.297	589.627	-153.992
250	303.401	530.779	595.672	-16.223	467.684	619.224	-129.377
298.15	370.248	589.952	589.952	0.000	461.814	648.959	-113.693
300	372.781	592.250	589.959	0.687	461.597	650.118	-113.193
350	439.302	654.763	594.744	21.006	456.194	681.978	-101.778
400	500.946	717.509	606.170	44.536	451.507	714.551	-93.309
450	556.796	779.795	622.008	71.004	447.447	747.680	-86.787
500	606.732	841.094	640.862	100.116	443.924	781.255	-81.615
600	690.470	959.420	684.182	165.143	438.179	849.290	-73.936
700	756.620	1071.020	731.556	237.625	433.966	918.169	-68.513
800	809.561	1175.635	780.600	316.028	431.116	987.539	-64.478
900	852.590	1273.556	829.992	399.207	429.453	1057.187	-61.356
1000	888.037	1365.278	878.984	486.294	428.818	1126.977	-58.866
1100	917.559	1451.344	927.146	576.618	429.009	1196.801	-56.830
1200	942.367	1532.276	974.235	669.649	429.887	1266.556	-55.131
1300	963.371	1608.558	1020.123	764.965	431.264	1336.228	-53.689
1400	981.271	1680.624	1064.752	862.220	433.008	1405.784	-52.449
1500	996.618	1748.861	1108.105	961.134	435.037	1475.208	-51.370
1600	1009.849	1813.614	1150.193	1061.473	437.219	1544.480	-50.421
1700	1021.318	1875.188	1191.044	1163.045	439.479	1613.587	-49.578
1800	1031.307	1933.854	1230.694	1265.688	441.739	1682.630	-48.828
1900	1040.050	1989.853	1269.188	1369.265	443.970	1751.491	-48.151
2000	1047.736	2043.401	1306.569	1473.662	446.118	1820.265	-47.539
2100	1054.523	2094.687	1342.886	1578.782	448.100	1888.920	-46.983
2200	1060.540	2143.885	1378.185	1684.541	449.917	1957.486	-46.476
2300	1065.895	2191.149	1412.510	1790.868	451.566	2025.974	-46.010
2400	1070.680	2236.616	1445.907	1897.701	452.971	2094.341	-45.581
2500	1074.969	2280.412	1478.416	2004.988	454.147	2162.778	-45.188
2600	1078.827	2322.649	1510.080	2112.681	455.056	2231.046	-44.821
2700	1082.308	2363.431	1540.934	2220.740	455.704	2299.365	-44.483
2800	1085.459	2402.850	1571.017	2329.131	456.063	2367.686	-44.169
2900	1088.319	2440.990	1600.362	2437.823	456.102	2435.942	-43.875
3000	1090.922	2477.931	1629.002	2546.787	455.870	2504.232	-43.602
3100	1093.298	2513.741	1656.967	2655.999	455.283	2572.449	-43.345
3200	1095.471	2548.487	1684.287	2765.439	454.387	2640.772	-43.105
3300	1097.464	2582.227	1710.989	2875.088	453.163	2709.171	-42.882
3400	1099.295	2615.017	1737.098	2984.927	451.580	2777.516	-42.670
3500	1100.982	2646.908	1762.639	3094.942	449.645	2845.893	-42.472
3600	1102.539	2677.946	1787.635	3205.119	447.382	2914.428	-42.286
3700	1103.978	2708.174	1812.108	3315.446	444.757	2983.046	-42.112
3800	1105.312	2737.633	1836.077	3425.911	441.743	3051.678	-41.947
3900	1106.550	2766.360	1859.564	3536.505	438.382	3120.333	-41.791
4000	1107.701	2794.390	1882.586	3647.218	434.660	3189.234	-41.646
4100	1108.772	2821.756	1905.160	3758.042	430.536	3258.151	-41.509
4200	1109.772	2848.486	1927.303	3868.970	426.042	3327.164	-41.378
4300	1110.705	2874.611	1949.031	3979.994	421.162	3396.190	-41.255
4400	1111.578	2900.156	1970.358	4091.109	415.907	3465.433	-41.139
4500	1112.396	2925.145	1991.299	4202.308	410.292	3534.861	-41.031
4600	1113.164	2949.603	2011.867	4313.587	404.260	3604.429	-40.929
4700	1113.884	2973.551	2032.074	4424.939	397.829	3674.007	-40.831
4800	1114.562	2997.009	2051.934	4536.362	391.048	3743.843	-40.740
4900	1115.200	3019.997	2071.456	4647.851	383.836	3813.674	-40.653
5000	1115.801	3042.533	2090.653	4759.401	376.296	3883.860	-40.574

3.433. Benzo[*rst*]naphtho[8,1,2-*cde*]pentaphene



Formula: C₃₀H₁₆
Mass: 376.448 g/mol
CAS Number: 52879-10-4
Point Group: C_s

Length: 18.01 Å
Width: 9.201 Å
Breadth: 3.886 Å
L/B Ratio: 1.957

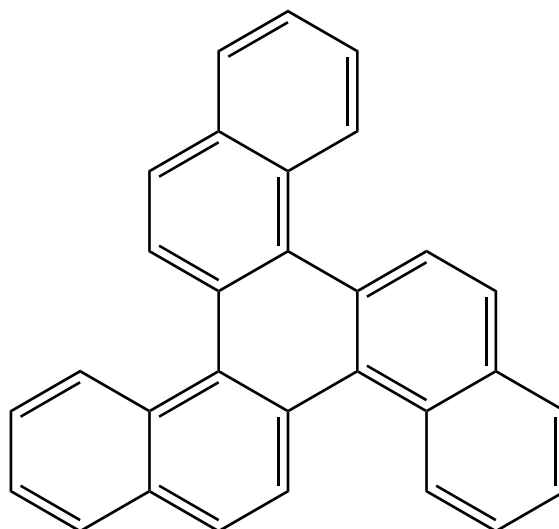
Cartesian coordinates:

C	6.3453	-1.6018	0.0000	C	2.6983	-0.7726	0.0000	H	6.5373	1.8060	0.0000
C	6.9121	-0.3077	0.0000	C	-1.7555	1.2700	0.0000	H	4.5287	-2.7619	0.0000
C	6.1056	0.7986	0.0000	C	-2.6256	2.4212	0.0000	H	4.3125	2.7984	0.0000
C	4.9853	-1.7603	0.0000	C	-3.9703	2.2967	0.0000	H	2.0893	3.8170	0.0000
C	4.1233	-0.6321	0.0000	C	-4.5940	0.9974	0.0000	H	-0.3796	3.5790	0.0000
C	4.6914	0.6585	0.0000	C	-5.9819	0.8554	0.0000	H	0.2573	-3.1874	0.0000
C	3.8522	1.8025	0.0000	C	-6.5575	-0.4125	0.0000	H	2.7410	-2.9454	0.0000
C	2.4831	1.6685	0.0000	C	-5.7634	-1.5491	0.0000	H	-2.1483	3.4132	0.0000
C	1.6186	2.8270	0.0000	C	-2.3424	-0.0231	0.0000	H	-4.6197	3.1797	0.0000
C	0.2775	2.6957	0.0000	C	-3.7714	-0.1540	0.0000	H	-6.6196	1.7466	0.0000
C	-0.3604	1.3989	0.0000	C	-4.3668	-1.4347	0.0000	H	-7.6483	-0.5109	0.0000
C	1.8859	0.3672	0.0000	C	-3.5195	-2.5951	0.0000	H	-6.2239	-2.5435	0.0000
C	0.4567	0.2383	0.0000	C	-2.1715	-2.4680	0.0000	H	-3.9934	-3.5833	0.0000
C	-0.1260	-1.0468	0.0000	C	-1.5375	-1.1780	0.0000	H	-1.5178	-3.3539	0.0000
C	0.7312	-2.1938	0.0000	H	7.0061	-2.4747	0.0000				
C	2.0819	-2.0636	0.0000	H	8.0019	-0.2021	0.0000				

Table 3.433: Table of thermodynamic data as a function of temperature for Benzo[*rst*]naphtho[8,1,2-*cde*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-53.735	470.599	470.599	∞
100	114.913	362.114	828.897	-46.678	497.395	544.621	-284.475
200	233.716	476.221	623.908	-29.537	483.204	597.511	-156.051
250	302.128	535.676	600.282	-16.152	476.542	626.858	-130.972
298.15	368.571	594.588	594.588	0.000	470.599	656.362	-114.990
300	371.092	596.875	594.595	0.684	470.380	657.513	-114.481
350	437.377	659.108	599.358	20.912	464.886	689.149	-102.848
400	498.921	721.589	610.733	44.342	460.100	721.511	-94.218
450	554.761	783.635	626.504	70.709	455.938	754.443	-87.572
500	604.742	844.722	645.281	99.720	452.314	787.831	-82.302
600	688.641	962.699	688.439	164.556	446.377	855.522	-74.478
700	754.974	1074.031	735.654	236.864	441.991	924.086	-68.955
800	808.083	1178.437	784.548	315.111	438.985	993.166	-64.846
900	851.258	1276.193	833.804	398.150	437.182	1062.542	-61.667
1000	886.834	1367.781	882.671	485.110	436.420	1132.076	-59.132
1100	916.470	1453.737	930.720	575.319	436.497	1201.655	-57.061
1200	941.378	1534.579	977.707	668.247	437.270	1271.175	-55.332
1300	962.469	1610.785	1023.502	763.468	438.553	1340.622	-53.866
1400	980.448	1682.787	1068.046	860.637	440.211	1409.958	-52.605
1500	995.865	1750.970	1111.322	959.472	442.162	1479.168	-51.508
1600	1009.160	1815.677	1153.340	1059.740	444.271	1548.231	-50.544
1700	1020.684	1877.211	1194.125	1161.245	446.465	1617.134	-49.687
1800	1030.724	1935.842	1233.716	1263.827	448.664	1685.977	-48.925
1900	1039.512	1991.811	1272.154	1367.348	450.840	1754.641	-48.237
2000	1047.239	2045.332	1309.485	1471.694	452.935	1823.220	-47.617
2100	1054.062	2096.595	1345.754	1576.766	454.869	1891.683	-47.052
2200	1060.112	2145.773	1381.009	1682.481	456.642	1960.059	-46.537
2300	1065.497	2193.017	1415.293	1788.766	458.250	2028.360	-46.065
2400	1070.308	2238.468	1448.651	1895.561	459.616	2096.541	-45.629
2500	1074.622	2282.249	1481.125	2002.811	460.757	2164.793	-45.230
2600	1078.502	2324.474	1512.754	2110.471	461.632	2232.878	-44.858
2700	1082.004	2365.243	1543.577	2218.499	462.249	2301.015	-44.515
2800	1085.173	2404.652	1573.630	2326.861	462.578	2369.155	-44.196
2900	1088.050	2442.783	1602.947	2435.524	462.590	2437.232	-43.898
3000	1090.669	2479.714	1631.560	2544.462	462.332	2505.343	-43.621
3100	1093.059	2515.517	1659.500	2653.650	461.720	2573.382	-43.360
3200	1095.246	2550.255	1686.796	2763.067	460.801	2641.527	-43.118
3300	1097.250	2583.989	1713.475	2872.693	459.555	2709.751	-42.891
3400	1099.093	2616.772	1739.563	2982.512	457.951	2777.919	-42.677
3500	1100.790	2648.657	1765.084	3092.507	455.997	2846.121	-42.475
3600	1102.357	2679.690	1790.060	3202.666	453.715	2914.482	-42.287
3700	1103.805	2709.913	1814.515	3312.975	451.072	2982.926	-42.110
3800	1105.147	2739.368	1838.467	3423.423	448.041	3051.383	-41.943
3900	1106.393	2768.091	1861.937	3534.001	444.664	3119.866	-41.785
4000	1107.551	2796.117	1884.942	3644.699	440.926	3188.594	-41.638
4100	1108.629	2823.479	1907.501	3755.508	436.788	3257.339	-41.498
4200	1109.635	2850.206	1929.630	3866.422	432.280	3326.179	-41.366
4300	1110.574	2876.328	1951.343	3977.433	427.387	3395.033	-41.241
4400	1111.453	2901.869	1972.657	4088.535	422.118	3464.105	-41.123
4500	1112.276	2926.856	1993.585	4199.722	416.491	3533.361	-41.013
4600	1113.049	2951.311	2014.140	4310.989	410.448	3602.759	-40.910
4700	1113.774	2975.257	2034.335	4422.330	404.005	3672.166	-40.811
4800	1114.456	2998.713	2054.183	4533.742	397.213	3741.831	-40.719
4900	1115.098	3021.699	2073.695	4645.220	389.991	3811.492	-40.630
5000	1115.703	3044.233	2092.881	4756.760	382.442	3881.508	-40.549

3.434. Benzo[*c*]naphtho[2,1-*p*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 27798-46-5
Point Group: C₃

Length: 14.16 Å
Width: 13.46 Å
Breadth: 6.015 Å
L/B Ratio: 1.053

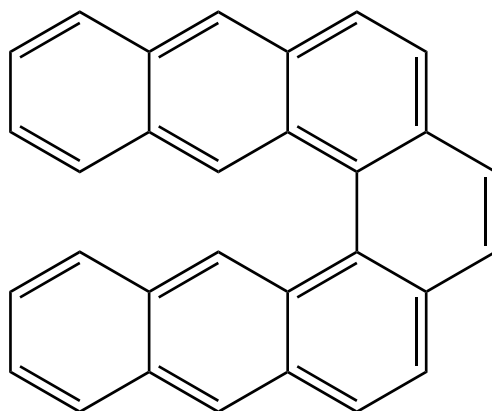
Cartesian coordinates:

C	-3.7396	3.3884	-0.5235	C	3.7141	-0.8556	-0.5629	H	-2.1435	5.2432	1.8214
C	-1.4322	3.3797	1.0335	C	5.0666	-0.6975	-0.7345	H	-4.1632	5.2936	0.3754
C	-2.3234	4.4221	1.1195	C	5.6815	0.5394	-0.4644	H	-4.0599	1.1865	-2.0322
C	-3.4761	4.4436	0.3143	C	4.9128	1.6051	-0.0726	H	-2.7561	-0.9048	-1.7783
C	-1.6444	2.3019	0.1402	C	0.7808	-1.1865	0.1578	H	3.2054	3.5704	0.5250
C	-2.8489	2.2920	-0.5926	C	-0.5871	-1.2656	-0.1221	H	0.7608	3.4168	0.5096
C	-3.1882	1.1426	-1.3698	C	0.8639	-3.5603	0.6783	H	3.2584	-1.8303	-0.7836
C	-2.4599	0.0046	-1.2376	C	1.4782	-2.3533	0.5954	H	5.6784	-1.5346	-1.0868
C	-0.7380	1.1796	0.0141	C	-0.5232	-3.6799	0.3775	H	6.7646	0.6434	-0.5840
C	-1.2737	-0.0325	-0.4404	C	-1.2660	-2.5353	0.0180	H	5.3690	2.5836	0.1166
C	0.6931	1.2509	0.2033	C	-2.6680	-2.7031	-0.1259	H	1.4153	-4.4513	1.0004
C	1.4647	0.0881	0.0804	C	-3.2672	-3.9302	0.0063	H	2.5381	-2.2655	0.8707
C	2.7112	2.6057	0.3613	C	-2.5008	-5.0730	0.3020	H	-3.3011	-1.8327	-0.3459
C	1.3579	2.5054	0.3711	C	-1.1499	-4.9455	0.4942	H	-4.3512	-4.0289	-0.1136
C	3.5118	1.4619	0.0765	H	-4.6481	3.3745	-1.1363	H	-2.9909	-6.0480	0.3872
C	2.8925	0.2097	-0.1120	H	-0.5458	3.3732	1.6827	H	-0.5373	-5.8185	0.7472

Table 3.434: Table of thermodynamic data as a function of temperature for Benzo[*c*]naphtho[2,1-*p*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.721	567.778	567.778	∞
100	124.641	359.114	851.143	-49.203	597.517	655.116	-342.190
200	246.084	480.813	635.577	-30.953	581.741	719.012	-187.783
250	316.517	543.232	610.836	-16.901	574.349	754.186	-157.575
298.15	385.351	604.879	604.879	0.000	567.778	789.435	-138.303
300	387.966	607.271	604.886	0.715	567.536	790.809	-137.689
350	456.769	672.295	609.865	21.851	561.501	828.512	-123.646
400	520.607	737.519	621.747	46.309	556.286	867.012	-113.218
450	578.434	802.237	638.213	73.811	551.799	906.127	-105.178
500	630.106	865.908	657.810	104.049	547.939	945.732	-98.798
600	716.712	988.760	702.822	171.563	541.752	1025.906	-89.311
700	785.187	1104.585	752.030	246.788	537.345	1106.977	-82.602
800	840.129	1213.148	802.959	328.151	534.501	1188.552	-77.603
900	884.944	1314.774	854.244	414.477	533.011	1270.395	-73.730
1000	922.010	1409.991	905.109	504.882	532.690	1352.353	-70.638
1100	953.001	1499.364	955.112	598.677	533.314	1434.307	-68.108
1200	979.136	1583.438	1004.004	695.320	534.725	1516.148	-65.995
1300	1001.333	1662.711	1051.654	794.373	536.719	1597.859	-64.201
1400	1020.303	1737.630	1098.001	895.480	539.150	1679.404	-62.658
1500	1036.607	1808.593	1143.030	998.345	541.923	1760.765	-61.314
1600	1050.692	1875.955	1186.750	1102.727	544.896	1841.922	-60.131
1700	1062.923	1940.028	1229.192	1208.422	547.985	1922.863	-59.081
1800	1073.593	2001.092	1270.392	1315.260	551.107	2003.692	-58.144
1900	1082.944	2059.394	1310.396	1423.097	554.226	2084.290	-57.300
2000	1091.175	2115.156	1349.250	1531.811	557.280	2164.753	-56.536
2100	1098.451	2168.574	1387.003	1641.300	560.185	2245.051	-55.841
2200	1104.907	2219.826	1423.701	1751.474	562.938	2325.218	-55.207
2300	1110.657	2269.070	1459.393	1862.258	565.533	2405.261	-54.624
2400	1115.798	2316.450	1494.123	1973.585	567.891	2485.143	-54.087
2500	1120.410	2362.094	1527.934	2085.400	570.026	2565.058	-53.593
2600	1124.561	2406.120	1560.869	2197.652	571.896	2644.762	-53.133
2700	1128.308	2448.633	1592.966	2310.299	573.507	2724.479	-52.707
2800	1131.701	2489.729	1624.264	2423.302	574.829	2804.167	-52.311
2900	1134.783	2529.496	1654.797	2536.628	575.829	2883.753	-51.941
3000	1137.588	2568.015	1684.599	2650.249	576.557	2963.339	-51.595
3100	1140.150	2605.359	1713.701	2764.138	576.926	3042.821	-51.270
3200	1142.493	2641.595	1742.135	2878.272	576.982	3122.378	-50.967
3300	1144.643	2676.784	1769.927	2992.630	576.704	3201.981	-50.682
3400	1146.619	2710.985	1797.104	3107.195	576.063	3281.503	-50.413
3500	1148.440	2744.250	1823.693	3221.949	575.062	3361.029	-50.160
3600	1150.120	2776.626	1849.715	3336.878	573.726	3440.683	-49.922
3700	1151.675	2808.160	1875.195	3451.969	572.021	3520.401	-49.698
3800	1153.115	2838.892	1900.153	3567.209	569.916	3600.101	-49.486
3900	1154.452	2868.862	1924.609	3682.588	567.458	3679.805	-49.284
4000	1155.695	2898.106	1948.582	3798.096	564.628	3759.731	-49.096
4100	1156.853	2926.658	1972.091	3913.724	561.388	3839.650	-48.917
4200	1157.933	2954.548	1995.152	4029.464	557.766	3919.643	-48.747
4300	1158.942	2981.807	2017.782	4145.309	553.749	3999.627	-48.585
4400	1159.886	3008.461	2039.995	4261.251	549.346	4079.811	-48.433
4500	1160.770	3034.537	2061.808	4377.284	544.572	4160.163	-48.289
4600	1161.600	3060.059	2083.232	4493.403	539.371	4240.632	-48.153
4700	1162.379	3085.049	2104.283	4609.602	533.758	4321.093	-48.023
4800	1163.112	3109.529	2124.971	4725.877	527.786	4401.795	-47.900
4900	1163.802	3133.519	2145.310	4842.223	521.372	4482.475	-47.783
5000	1164.452	3157.037	2165.310	4958.636	514.620	4563.499	-47.674

3.435. Benzo[2,1-*a*:3,4-*a'*]dianthracene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 188-51-2
Point Group: C₂

Length: 13.39 Å
Width: 12.61 Å
Breadth: 6.957 Å
L/B Ratio: 1.062

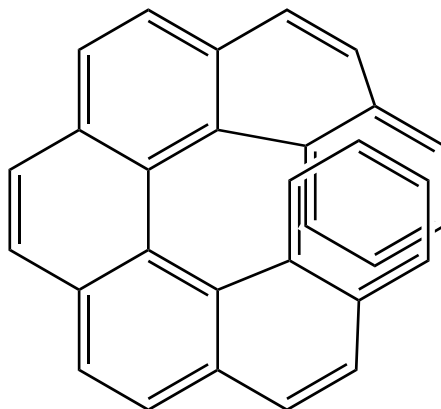
Cartesian coordinates:

C	4.2221	2.5648	-0.1259	C	-0.6056	-4.3631	-0.3148	H	-0.8900	2.5765	2.1517
C	3.3589	1.4291	-0.0590	C	0.6092	-4.3625	0.3171	H	-5.1606	2.5421	-0.4443
C	2.1462	1.4393	-0.7873	C	-1.5739	-0.7633	-0.0881	H	-0.3403	0.3613	1.2822
C	1.8276	2.5780	-1.5889	C	-2.8459	-0.8092	-0.7326	H	-4.6646	0.2491	-1.2075
C	2.6752	3.6449	-1.6377	C	-3.2810	-2.0340	-1.3570	H	-2.9124	-4.1196	-1.6140
C	3.8862	3.6398	-0.8941	C	-2.5566	-3.1630	-1.2138	H	-4.2324	-2.0313	-1.9010
C	1.2749	0.3388	-0.7049	C	-1.2753	0.3378	0.7048	H	1.0933	-5.3032	0.6031
C	1.5747	-0.7617	0.0884	C	-2.1479	1.4373	0.7871	H	-1.0892	-5.3045	-0.5997
C	2.8468	-0.8062	0.7328	C	-3.3617	1.4248	0.0606	H	4.2371	-2.0277	1.8966
C	3.6999	0.2875	0.6852	C	-3.7012	0.2827	-0.6835	H	2.9194	-4.1178	1.6091
C	0.6944	-1.9207	0.1766	C	-1.8290	2.5775	1.5864	H	0.3403	0.3610	-1.2827
C	1.2763	-3.1394	0.5596	C	-2.6778	3.6435	1.6353	H	4.6628	0.2558	1.2101
C	2.5612	-3.1610	1.2117	C	-3.8904	3.6355	0.8946	H	0.8898	2.5750	-2.1564
C	3.2845	-2.0312	1.3548	C	-4.2266	2.5590	0.1284	H	2.4356	4.5208	-2.2494
C	-0.6924	-1.9214	-0.1760	H	-4.5490	4.5083	0.9518	H	4.5435	4.5136	-0.9507
C	-1.2730	-3.1406	-0.5590	H	-2.4374	4.5212	2.2441	H	5.1547	2.5497	0.4493

Table 3.435: Table of thermodynamic data as a function of temperature for Benzo[2,1-*a*:3,4-*a'*]dianthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.944	546.468	546.468	∞
100	124.537	367.137	859.945	-49.281	576.129	632.926	-330.600
200	246.581	488.826	643.966	-31.028	560.356	696.024	-181.779
250	317.334	551.397	619.165	-16.942	552.998	730.794	-152.688
298.15	386.193	613.193	613.193	0.000	546.468	765.646	-134.135
300	388.805	615.590	613.201	0.717	546.228	767.004	-133.545
350	457.447	680.733	618.189	21.891	540.231	804.289	-120.031
400	521.062	746.033	630.090	46.377	535.044	842.364	-109.999
450	578.677	810.792	646.578	73.896	530.574	881.053	-102.268
500	630.181	874.480	666.195	104.143	526.723	920.229	-96.134
600	716.600	997.326	711.238	171.653	520.532	999.546	-87.016
700	785.034	1113.129	760.466	246.864	516.111	1079.761	-80.571
800	840.009	1221.673	811.408	328.212	513.252	1160.483	-75.770
900	884.885	1323.289	862.700	414.530	511.754	1241.474	-72.052
1000	922.014	1418.502	913.571	504.932	511.430	1322.581	-69.083
1100	953.059	1507.879	963.578	598.731	512.057	1403.684	-66.654
1200	979.236	1591.960	1012.475	695.382	513.477	1484.673	-64.625
1300	1001.463	1671.242	1060.129	794.446	515.482	1565.532	-62.903
1400	1020.454	1746.171	1106.481	895.567	517.926	1646.223	-61.420
1500	1036.771	1817.146	1151.514	998.448	520.716	1726.728	-60.129
1600	1050.864	1884.518	1195.239	1102.847	523.706	1807.030	-58.992
1700	1063.097	1948.602	1237.685	1208.559	526.812	1887.114	-57.983
1800	1073.767	2009.676	1278.890	1315.414	529.951	1967.086	-57.082
1900	1083.115	2067.987	1318.899	1423.268	533.087	2046.824	-56.270
2000	1091.342	2123.757	1357.758	1532.000	536.159	2126.428	-55.535
2100	1098.613	2177.184	1395.515	1641.505	539.080	2205.865	-54.867
2200	1105.063	2228.443	1432.218	1751.695	541.849	2285.171	-54.256
2300	1110.808	2277.694	1467.914	1862.494	544.459	2364.352	-53.695
2400	1115.942	2325.080	1502.648	1973.836	546.832	2443.372	-53.178
2500	1120.548	2370.730	1536.464	2085.665	548.981	2522.423	-52.702
2600	1124.693	2414.761	1569.403	2197.930	550.864	2601.263	-52.259
2700	1128.434	2457.279	1601.505	2310.590	552.488	2680.116	-51.849
2800	1131.822	2498.379	1632.806	2423.605	553.822	2758.939	-51.468
2900	1134.898	2538.151	1663.343	2536.944	554.835	2837.660	-51.111
3000	1137.698	2576.674	1693.149	2650.576	555.574	2916.379	-50.778
3100	1140.254	2614.021	1722.255	2764.475	555.953	2994.996	-50.464
3200	1142.593	2650.260	1750.691	2878.619	556.019	3073.686	-50.172
3300	1144.739	2685.453	1778.487	2992.988	555.752	3152.423	-49.898
3400	1146.711	2719.656	1805.668	3107.561	555.119	3231.078	-49.638
3500	1148.527	2752.923	1832.259	3222.325	554.128	3309.736	-49.394
3600	1150.204	2785.302	1858.285	3337.262	552.800	3388.523	-49.165
3700	1151.755	2816.838	1883.767	3452.361	551.103	3467.373	-48.950
3800	1153.192	2847.573	1908.728	3567.609	549.006	3546.205	-48.745
3900	1154.526	2877.545	1933.187	3682.996	546.556	3625.041	-48.551
4000	1155.766	2906.791	1957.163	3798.511	543.733	3704.099	-48.370
4100	1156.921	2935.344	1980.674	3914.146	540.499	3783.149	-48.197
4200	1157.998	2963.236	2003.738	4029.893	536.885	3862.273	-48.033
4300	1159.004	2990.496	2026.370	4145.744	532.874	3941.389	-47.877
4400	1159.946	3017.152	2048.586	4261.692	528.477	4020.704	-47.731
4500	1160.828	3043.229	2070.400	4377.731	523.709	4100.186	-47.593
4600	1161.655	3068.752	2091.827	4493.856	518.513	4179.786	-47.462
4700	1162.432	3093.743	2112.879	4610.060	512.906	4259.378	-47.337
4800	1163.163	3118.224	2133.570	4726.340	506.939	4339.210	-47.219
4900	1163.851	3142.215	2153.911	4842.692	500.530	4419.021	-47.106
5000	1164.500	3165.735	2173.913	4959.109	493.783	4499.176	-47.002

3.436. Dinaphtho[2,1-c 1',2'-g]phenanthrene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 16914-68-4
Point Group: C₂

Length: 11.66 Å
Width: 10.51 Å
Breadth: 8.920 Å
L/B Ratio: 1.109

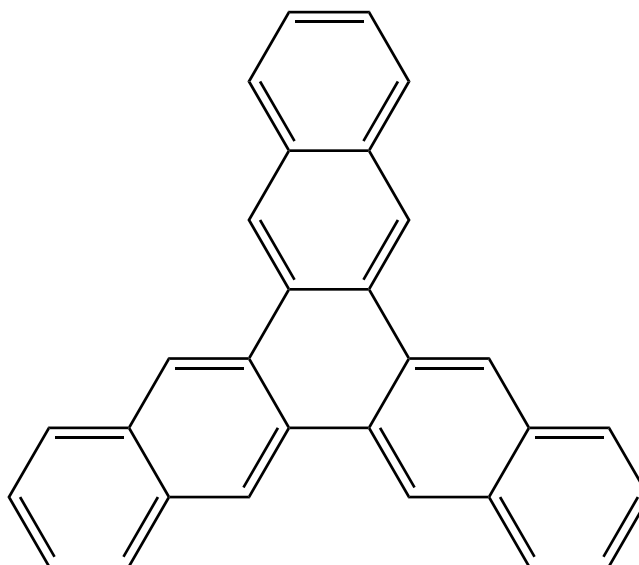
Cartesian coordinates:

C	3.0033	-1.6227	1.9372	C	-2.8045	1.2364	0.3811	H	-1.4207	-4.4674	-1.3341
C	1.9195	-1.9904	1.1067	C	-1.5655	0.6622	0.0463	H	-3.5999	-3.2677	-1.1637
C	0.7436	-1.2122	1.0893	C	-2.8726	2.5818	0.8417	H	-4.8765	-1.3481	-0.4581
C	0.6440	-0.1463	2.0145	C	-1.7416	3.3369	0.9057	H	-4.9652	0.9691	0.4631
C	1.6925	0.1772	2.8425	C	-0.5290	2.8486	0.3406	H	-3.8397	2.9815	1.1670
C	2.8949	-0.5490	2.7865	C	-0.4681	1.5617	-0.2147	H	-1.7589	4.3447	1.3360
C	-0.3464	-1.5937	0.2161	C	0.6167	3.7070	0.3196	H	0.5619	4.6619	0.8550
C	-0.3082	-2.8809	-0.3405	C	1.7435	3.3379	-0.3372	H	2.6396	3.9685	-0.3268
C	0.9004	-3.6482	-0.3211	C	1.7583	2.1331	-1.1102	H	3.7368	2.5153	-1.9127
C	1.9965	-3.1926	0.3334	C	0.6470	1.2653	-1.0894	H	3.6944	0.5499	-3.4388
C	-1.4804	-3.4612	-0.9039	C	2.8655	1.8512	-1.9434	H	1.6669	-0.8814	-3.5522
C	-2.6661	-2.7954	-0.8383	C	2.8400	0.7711	-2.7913	H	-0.2565	-0.4508	-2.0729
C	-2.7016	-1.4490	-0.3770	C	1.6986	-0.0478	-2.8430	H	-0.2904	0.4257	2.0773
C	-1.5102	-0.7813	-0.0427	C	0.6298	0.1934	-2.0130	H	1.5967	1.0045	3.5533
C	-3.9604	-0.7905	-0.2328	H	0.9181	-4.6053	-0.8548	H	3.7310	-0.2618	3.4319
C	-4.0091	0.4831	0.2380	H	2.9389	-3.7517	0.3210	H	3.9244	-2.2156	1.9030

Table 3.436: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1-*c*1',2'-*g*]phenanthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.869	571.972	571.972	∞
100	124.437	360.457	853.294	-49.284	601.630	659.095	-344.269
200	246.545	482.049	637.271	-31.045	585.843	722.867	-188.790
250	317.500	544.632	612.454	-16.956	578.488	757.975	-158.367
298.15	386.593	606.477	606.477	0.000	571.972	793.152	-138.954
300	389.214	608.877	606.485	0.718	571.732	794.523	-138.336
350	458.096	674.101	611.478	21.918	565.762	832.141	-124.188
400	521.905	739.501	623.396	46.442	560.613	870.546	-113.679
450	579.655	804.368	639.908	74.007	556.189	909.559	-105.577
500	631.236	868.163	659.554	104.304	552.388	949.053	-99.145
600	717.676	991.205	704.669	171.922	546.305	1028.991	-89.580
700	786.031	1107.169	753.973	247.237	541.988	1109.811	-82.813
800	840.891	1215.839	804.989	328.680	539.224	1191.122	-77.771
900	885.647	1317.552	856.352	415.080	537.808	1272.691	-73.864
1000	922.666	1412.840	907.287	505.552	537.554	1354.368	-70.743
1100	953.616	1502.273	957.354	599.411	538.242	1436.034	-68.190
1200	979.712	1586.399	1006.304	696.114	539.713	1517.582	-66.057
1300	1001.873	1665.717	1054.007	795.223	541.763	1598.994	-64.247
1400	1020.808	1740.675	1100.402	896.381	544.245	1680.236	-62.689
1500	1037.078	1811.672	1145.475	999.296	547.067	1761.291	-61.332
1600	1051.133	1879.063	1189.236	1103.723	550.086	1842.139	-60.138
1700	1063.334	1943.162	1231.715	1209.460	553.217	1922.768	-59.078
1800	1073.976	2004.249	1272.950	1316.338	556.379	2003.282	-58.133
1900	1083.302	2062.571	1312.986	1424.212	559.535	2083.563	-57.280
2000	1091.509	2118.350	1351.869	1532.961	562.624	2163.708	-56.509
2100	1098.763	2171.784	1389.650	1642.482	565.561	2243.685	-55.807
2200	1105.199	2223.050	1426.374	1752.686	568.344	2323.531	-55.166
2300	1110.931	2272.307	1462.090	1863.498	570.967	2403.251	-54.578
2400	1116.055	2319.698	1496.843	1974.852	573.352	2482.809	-54.036
2500	1120.651	2365.352	1530.676	2086.692	575.511	2562.398	-53.537
2600	1124.787	2409.387	1563.630	2198.967	577.405	2641.776	-53.073
2700	1128.522	2451.908	1595.747	2311.636	579.038	2721.166	-52.643
2800	1131.903	2493.012	1627.062	2424.660	580.380	2800.526	-52.243
2900	1134.973	2532.786	1657.612	2538.006	581.401	2879.783	-51.869
3000	1137.768	2571.311	1687.430	2651.645	582.147	2959.040	-51.520
3100	1140.319	2608.661	1716.547	2765.551	582.533	3038.192	-51.192
3200	1142.654	2644.902	1744.995	2879.702	582.605	3117.419	-50.886
3300	1144.796	2680.097	1772.801	2994.076	582.343	3196.691	-50.598
3400	1146.764	2714.302	1799.991	3108.655	581.717	3275.881	-50.327
3500	1148.577	2747.570	1826.592	3223.423	580.730	3355.075	-50.071
3600	1150.251	2779.950	1852.626	3338.366	579.408	3434.397	-49.831
3700	1151.799	2811.487	1878.117	3453.469	577.715	3513.782	-49.605
3800	1153.234	2842.223	1903.086	3568.722	575.623	3593.149	-49.390
3900	1154.565	2872.196	1927.552	3684.113	573.177	3672.521	-49.187
4000	1155.803	2901.443	1951.535	3799.632	570.358	3752.113	-48.997
4100	1156.957	2929.997	1975.053	3915.271	567.127	3831.698	-48.815
4200	1158.032	2957.890	1998.123	4031.021	563.516	3911.356	-48.644
4300	1159.037	2985.151	2020.762	4146.875	559.508	3991.006	-48.480
4400	1159.977	3011.808	2042.984	4262.826	555.115	4070.856	-48.326
4500	1160.857	3037.886	2064.804	4378.868	550.350	4150.873	-48.181
4600	1161.683	3063.409	2086.236	4494.996	545.157	4231.007	-48.044
4700	1162.459	3088.401	2107.294	4611.203	539.553	4311.133	-47.912
4800	1163.189	3112.883	2127.990	4727.486	533.589	4391.500	-47.788
4900	1163.876	3136.874	2148.335	4843.840	527.182	4471.845	-47.669
5000	1164.524	3160.394	2168.342	4960.260	520.438	4552.533	-47.559

3.437. Trinaphthylene



Other names: Naphtho[2,3-*h*]pentaphene
Dinaphth[2,3-*a*,2',3'-*c*]anthracene

Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 196-62-3
Point Group: D_{3h}

Length: 15.89 Å
Width: 14.10 Å
Breadth: 3.890 Å
L/B Ratio: 1.127

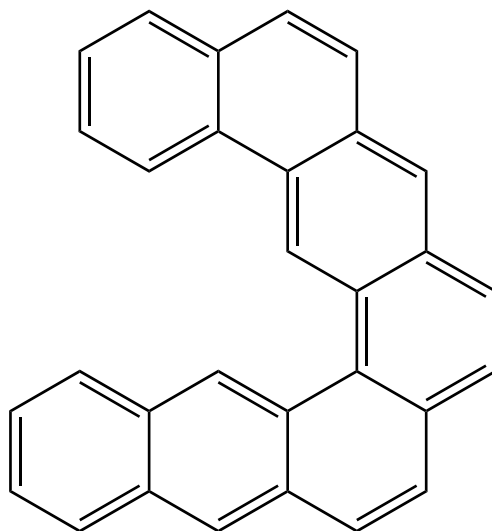
Cartesian coordinates:

C	-3.0286	-5.3568	0.0000	C	-1.8606	4.7806	0.0000	H	0.3866	-5.5092	0.0000
C	-1.7234	-5.9074	0.0000	C	-3.1248	5.3013	0.0000	H	-4.2159	-3.5676	0.0000
C	-0.6264	-5.0915	0.0000	C	-4.2542	4.4462	0.0000	H	1.3402	-3.2407	0.0000
C	-3.2098	-4.0017	0.0000	C	-4.0962	3.0883	0.0000	H	-3.2564	-1.3015	0.0000
C	-2.0853	-3.1294	0.0000	C	1.1583	0.8639	0.0000	H	0.5011	3.4709	0.0000
C	-0.7863	-3.6774	0.0000	C	1.3354	-0.5521	0.0000	H	-3.4766	0.4597	0.0000
C	0.3272	-2.8068	0.0000	C	2.6126	-1.0767	0.0000	H	-0.9817	5.4349	0.0000
C	-2.2388	-1.7243	0.0000	C	2.2671	1.6868	0.0000	H	-3.2805	6.3851	0.0000
C	-1.1459	-0.8804	0.0000	C	3.5779	1.1577	0.0000	H	-5.2551	4.8903	0.0000
C	0.1690	-1.4351	0.0000	C	3.7528	-0.2412	0.0000	H	-4.9645	2.4198	0.0000
C	-1.3273	0.5712	0.0000	C	5.0704	-0.7789	0.0000	H	2.7553	-2.1694	0.0000
C	-0.1895	1.4325	0.0000	C	6.1534	0.0555	0.0000	H	2.1364	2.7810	0.0000
C	-0.3739	2.8010	0.0000	C	5.9777	1.4611	0.0000	H	5.1976	-1.8673	0.0000
C	-2.5944	1.1200	0.0000	C	4.7226	2.0033	0.0000	H	7.1699	-0.3515	0.0000
C	-2.7916	2.5197	0.0000	H	-3.8893	-6.0336	0.0000	H	6.8627	2.1059	0.0000
C	-1.6675	3.3706	0.0000	H	-1.6075	-6.9962	0.0000	H	4.5779	3.0894	0.0000

Table 3.437: Table of thermodynamic data as a function of temperature for Trinaphthylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-57.740	499.269	499.269	∞
100	129.008	374.363	870.560	-49.620	528.591	584.665	-305.392
200	247.978	498.252	653.592	-31.068	513.117	646.900	-168.949
250	317.654	561.008	628.774	-16.941	505.800	681.193	-142.324
298.15	385.910	622.804	622.804	0.000	499.269	715.581	-125.364
300	388.505	625.200	622.812	0.716	499.028	716.922	-124.825
350	456.821	690.269	627.795	21.866	493.007	753.728	-112.485
400	520.282	755.473	639.682	46.317	487.785	791.329	-103.335
450	577.842	820.137	656.147	73.795	483.274	829.548	-96.289
500	629.343	883.736	675.737	104.000	479.381	868.259	-90.705
600	715.821	1006.434	720.720	171.429	473.109	946.658	-82.412
700	784.333	1122.123	769.886	246.566	468.614	1025.968	-76.557
800	839.382	1230.578	820.769	327.848	465.689	1105.796	-72.200
900	884.322	1332.124	872.006	414.106	464.131	1185.900	-68.826
1000	921.505	1427.281	922.827	504.454	463.753	1266.126	-66.134
1100	952.597	1516.611	972.789	598.205	464.333	1346.353	-63.932
1200	978.815	1600.654	1021.644	694.812	465.708	1426.471	-62.091
1300	1001.080	1679.904	1069.260	793.836	467.673	1506.462	-60.529
1400	1020.104	1754.806	1115.578	894.920	470.081	1586.288	-59.184
1500	1036.450	1825.757	1160.579	997.768	472.837	1665.932	-58.012
1600	1050.569	1893.110	1204.275	1102.135	475.795	1745.374	-56.979
1700	1062.826	1957.176	1246.694	1207.819	478.873	1824.599	-56.062
1800	1073.517	2018.235	1287.875	1314.649	481.987	1903.714	-55.243
1900	1082.885	2076.534	1327.861	1422.479	485.099	1982.597	-54.504
2000	1091.129	2132.293	1366.699	1531.188	488.148	2061.347	-53.836
2100	1098.414	2185.709	1404.436	1640.673	491.049	2139.931	-53.227
2200	1104.879	2236.959	1441.121	1750.844	493.799	2218.385	-52.670
2300	1110.636	2286.203	1476.800	1861.625	496.391	2296.715	-52.159
2400	1115.783	2333.582	1511.519	1972.950	498.747	2374.884	-51.687
2500	1120.399	2379.225	1545.320	2084.764	500.881	2453.085	-51.253
2600	1124.553	2423.250	1578.245	2197.015	502.750	2531.076	-50.849
2700	1128.303	2465.763	1610.333	2309.661	504.360	2609.080	-50.475
2800	1131.699	2506.859	1641.622	2422.664	505.682	2687.055	-50.127
2900	1134.782	2546.627	1672.147	2535.990	506.682	2764.928	-49.801
3000	1137.589	2585.145	1701.942	2649.611	507.410	2842.801	-49.497
3100	1140.151	2622.489	1731.038	2763.500	507.779	2920.570	-49.210
3200	1142.496	2658.725	1759.464	2877.634	507.835	2998.414	-48.943
3300	1144.647	2693.915	1787.251	2991.993	507.558	3076.304	-48.693
3400	1146.623	2728.116	1814.422	3106.557	506.916	3154.113	-48.456
3500	1148.445	2761.380	1841.005	3221.312	505.916	3231.925	-48.233
3600	1150.125	2793.757	1867.023	3336.242	504.581	3309.867	-48.024
3700	1151.680	2825.291	1892.498	3451.333	502.876	3387.871	-47.827
3800	1153.121	2856.023	1917.451	3566.574	500.772	3465.858	-47.641
3900	1154.458	2885.994	1941.903	3681.954	498.315	3543.850	-47.464
4000	1155.701	2915.238	1965.872	3797.462	495.485	3622.062	-47.298
4100	1156.859	2943.789	1989.377	3913.091	492.245	3700.268	-47.141
4200	1157.939	2971.680	2012.434	4028.831	488.624	3778.547	-46.992
4300	1158.948	2998.939	2035.061	4144.676	484.607	3856.818	-46.850
4400	1159.892	3025.593	2057.271	4260.619	480.205	3935.290	-46.717
4500	1160.776	3051.670	2079.080	4376.653	475.432	4013.928	-46.592
4600	1161.605	3077.191	2100.502	4492.772	470.231	4092.684	-46.473
4700	1162.385	3102.181	2121.549	4608.972	464.619	4171.432	-46.359
4800	1163.117	3126.661	2142.235	4725.248	458.648	4250.420	-46.253
4900	1163.807	3150.651	2162.571	4841.594	452.234	4329.388	-46.151
5000	1164.457	3174.170	2182.568	4958.008	445.483	4408.698	-46.056

3.438. Anthra[1,2-*a*]benz[*j*]anthracene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-59-6
Point Group: C₁

Length: 14.74 Å
Width: 12.43 Å
Breadth: 5.418 Å
L/B Ratio: 1.186

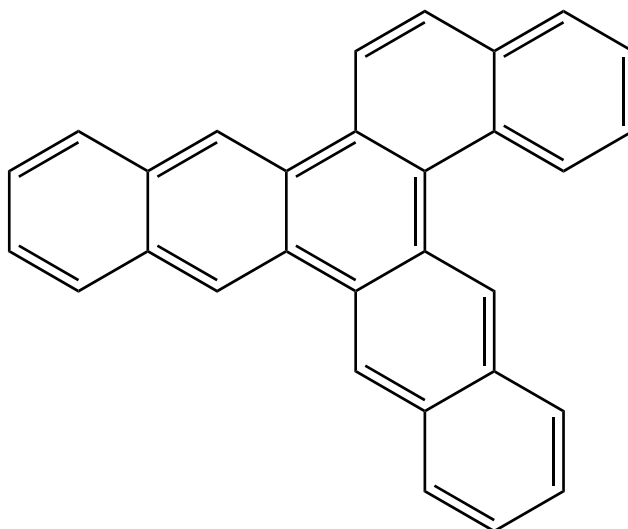
Cartesian coordinates:

C	4.3299	-3.5115	0.5889	C	-1.0563	1.7946	0.0399	H	1.2176	-2.1081	0.6723
C	5.0718	-2.3994	0.2495	C	-1.5385	3.0962	0.1598	H	2.3594	-4.2985	1.0117
C	2.3090	-2.1989	0.5564	C	-2.9057	3.3533	0.5171	H	6.2973	-0.1118	-0.4196
C	2.9406	-3.4105	0.7425	C	-3.7744	2.3353	0.7001	H	5.2062	2.0935	-0.7520
C	3.0478	-1.0504	0.2134	C	-2.0281	0.7097	0.0250	H	3.1993	3.4847	-0.6869
C	4.4408	-1.1554	0.0571	C	-3.3728	0.9838	0.4201	H	0.4421	-0.5084	0.4316
C	5.2142	0.0076	-0.3002	C	-4.3229	-0.0316	0.4725	H	1.2755	4.9121	-0.5606
C	4.6212	1.2070	-0.4811	C	-1.7404	-0.5760	-0.4273	H	-1.1288	5.2290	-0.0165
C	2.4014	0.2354	0.0140	C	-2.6959	-1.6023	-0.4021	H	-3.2174	4.3942	0.6636
C	3.1962	1.3601	-0.3214	C	-3.9995	-1.3369	0.0810	H	-4.8048	2.5181	1.0260
C	2.5875	2.6010	-0.4650	C	-4.9567	-2.3977	0.1284	H	-5.3446	0.1931	0.8039
C	1.0243	0.3850	0.1430	C	-4.6197	-3.6467	-0.2981	H	-0.7444	-0.8162	-0.8280
C	0.3797	1.6141	-0.0624	C	-3.3141	-3.9118	-0.7974	H	-5.9601	-2.1814	0.5121
C	1.2016	2.7456	-0.3096	C	-2.3785	-2.9231	-0.8503	H	-5.3469	-4.4645	-0.2653
C	0.6263	4.0567	-0.3414	H	4.8219	-4.4780	0.7395	H	-3.0767	-4.9251	-1.1376
C	-0.6876	4.2263	-0.0600	H	6.1584	-2.4744	0.1270	H	-1.3703	-3.1192	-1.2332

Table 3.438: Table of thermodynamic data as a function of temperature for Anthra[1,2-*a*]benz[*j*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.949	515.141	515.141	∞
100	124.838	374.853	867.386	-49.253	544.830	600.855	-313.848
200	246.397	496.611	651.578	-30.993	529.064	663.175	-173.200
250	316.964	559.118	626.805	-16.922	521.692	697.557	-145.744
298.15	385.735	620.841	620.841	0.000	515.141	732.039	-128.248
300	388.345	623.235	620.848	0.716	514.900	733.383	-127.691
350	456.966	688.305	625.831	21.866	508.879	770.287	-114.957
400	520.599	753.541	637.719	46.329	503.669	807.986	-105.510
450	578.249	818.248	654.191	73.826	499.177	846.301	-98.234
500	629.793	881.893	673.789	104.052	495.305	885.105	-92.464
600	716.281	1004.675	718.797	171.527	489.079	963.684	-83.894
700	784.764	1120.432	767.992	246.708	484.629	1043.167	-77.840
800	839.772	1228.943	818.903	328.032	481.745	1123.160	-73.333
900	884.672	1330.532	870.169	414.327	480.224	1203.426	-69.844
1000	921.818	1425.724	921.016	504.708	479.880	1283.810	-67.058
1100	952.877	1515.082	971.002	598.488	480.488	1364.191	-64.779
1200	979.067	1599.148	1019.880	695.122	481.890	1444.461	-62.874
1300	1001.306	1678.417	1067.517	794.170	483.879	1524.601	-61.258
1400	1020.308	1753.335	1113.853	895.275	486.308	1604.575	-59.866
1500	1036.634	1824.300	1158.871	998.142	489.084	1684.365	-58.654
1600	1050.737	1891.664	1202.584	1102.528	492.060	1763.952	-57.586
1700	1062.979	1955.740	1245.018	1208.228	495.154	1843.322	-56.637
1800	1073.656	2016.807	1286.212	1315.072	498.282	1922.580	-55.791
1900	1083.013	2075.113	1326.210	1422.915	501.407	2001.605	-55.027
2000	1091.246	2130.878	1365.060	1531.637	504.469	2080.497	-54.336
2100	1098.523	2184.300	1402.808	1641.133	507.381	2159.222	-53.707
2200	1104.979	2235.555	1439.503	1751.314	510.141	2237.816	-53.131
2300	1110.729	2284.803	1475.192	1862.105	512.743	2316.286	-52.603
2400	1115.869	2332.186	1509.919	1973.439	515.109	2394.595	-52.116
2500	1120.479	2377.833	1543.728	2085.261	517.250	2472.936	-51.668
2600	1124.628	2421.861	1576.661	2197.520	519.127	2551.066	-51.250
2700	1128.373	2464.376	1608.756	2310.173	520.744	2629.209	-50.864
2800	1131.764	2505.475	1640.052	2423.183	522.073	2707.323	-50.505
2900	1134.843	2545.244	1670.584	2536.516	523.080	2785.334	-50.168
3000	1137.647	2583.765	1700.385	2650.142	523.813	2863.345	-49.854
3100	1140.206	2621.111	1729.486	2764.037	524.188	2941.252	-49.559
3200	1142.547	2657.348	1757.918	2878.176	524.249	3019.234	-49.283
3300	1144.695	2692.540	1785.710	2992.540	523.977	3097.261	-49.025
3400	1146.669	2726.742	1812.886	3107.109	523.341	3175.208	-48.780
3500	1148.488	2760.008	1839.474	3221.868	522.345	3253.157	-48.550
3600	1150.167	2792.386	1865.496	3336.802	521.014	3331.236	-48.334
3700	1151.719	2823.920	1890.975	3451.898	519.313	3409.378	-48.131
3800	1153.158	2854.654	1915.932	3567.142	517.213	3487.501	-47.938
3900	1154.493	2884.625	1940.388	3682.526	514.759	3565.630	-47.755
4000	1155.735	2913.870	1964.361	3798.038	511.933	3643.979	-47.585
4100	1156.891	2942.423	1987.869	3913.670	508.696	3722.321	-47.422
4200	1157.970	2970.314	2010.930	4029.413	505.079	3800.738	-47.268
4300	1158.977	2997.574	2033.560	4145.261	501.065	3879.145	-47.121
4400	1159.920	3024.229	2055.773	4261.207	496.665	3957.753	-46.984
4500	1160.803	3050.306	2077.585	4377.243	491.895	4036.527	-46.854
4600	1161.631	3075.828	2099.010	4493.365	486.697	4115.420	-46.731
4700	1162.409	3100.819	2120.060	4609.568	481.087	4194.304	-46.613
4800	1163.141	3125.299	2140.748	4725.846	475.118	4273.429	-46.503
4900	1163.830	3149.290	2161.087	4842.195	468.707	4352.532	-46.398
5000	1164.479	3172.809	2181.087	4958.610	461.958	4431.979	-46.300

3.439. Naphtho[1,2-*h*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-64-3
Point Group: C₁

Length: 15.78 Å
Width: 13.14 Å
Breadth: 5.207 Å
L/B Ratio: 1.201

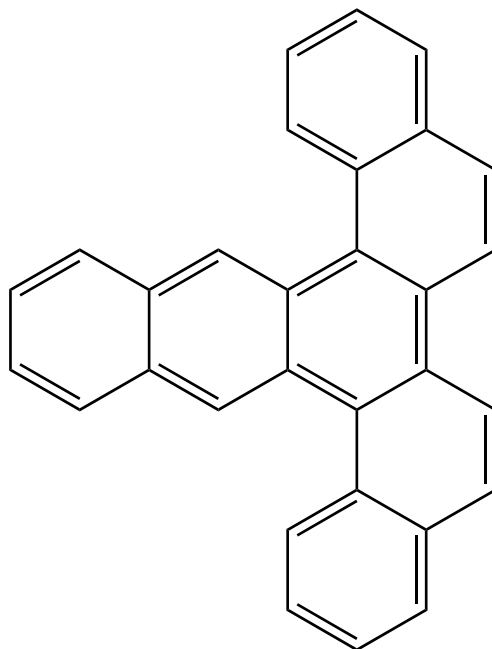
Cartesian coordinates:

C	6.2116	-0.8935	0.3524	C	-3.7101	-2.9829	-0.4442	H	5.3113	2.2984	-0.4795
C	6.3355	0.4765	0.0087	C	-3.8137	-4.3434	-0.3718	H	4.8735	-2.5299	0.7270
C	5.2241	1.2387	-0.2147	C	-2.6737	-5.1386	-0.0925	H	2.8669	2.4971	-0.5637
C	4.9788	-1.4717	0.4627	C	-1.4528	-4.5563	0.1001	H	2.4198	-2.3441	0.5616
C	3.8027	-0.7014	0.2333	C	-0.9675	1.1450	-0.0712	H	-3.2250	-0.3527	-0.4835
C	3.9254	0.6632	-0.1045	C	0.2931	1.6864	-0.3065	H	0.8331	-3.1240	0.3267
C	2.7592	1.4295	-0.3147	C	0.4304	3.0696	-0.6136	H	-4.5867	-2.3617	-0.6601
C	2.5158	-1.2726	0.3235	C	-0.6445	3.9042	-0.6035	H	-4.7782	-4.8376	-0.5280
C	1.3797	-0.5176	0.0988	C	-2.0713	2.0494	0.1319	H	-2.7879	-6.2261	-0.0355
C	1.4994	0.8698	-0.2001	C	-1.9105	3.4181	-0.1779	H	-0.5650	-5.1623	0.3124
C	0.0559	-1.1302	0.0989	C	-2.9924	4.3243	-0.0251	H	1.4281	3.4552	-0.8725
C	-1.1072	-0.3137	-0.0591	C	-4.1885	3.8983	0.4856	H	-0.5432	4.9590	-0.8834
C	-2.3195	-0.9426	-0.2786	C	-4.3377	2.5517	0.8767	H	-2.8483	5.3720	-0.3133
C	-0.0656	-2.5053	0.1715	C	-3.3131	1.6590	0.7037	H	-5.0265	4.5920	0.6075
C	-1.3160	-3.1409	0.0243	H	7.1198	-1.4796	0.5273	H	-5.2820	2.2275	1.3265
C	-2.4515	-2.3481	-0.2378	H	7.3364	0.9128	-0.0740	H	-3.4527	0.6174	1.0240

Table 3.439: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*h*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.005	521.362	521.362	∞
100	126.415	373.958	866.911	-49.295	551.009	607.124	-317.122
200	246.442	496.400	651.131	-30.946	535.332	669.486	-174.848
250	316.432	558.850	626.402	-16.888	527.946	703.879	-147.064
298.15	384.901	620.450	620.450	0.000	521.362	738.377	-129.358
300	387.503	622.839	620.458	0.714	521.120	739.722	-128.794
350	455.990	687.767	625.429	21.818	515.053	776.649	-115.906
400	519.591	752.871	637.292	46.231	509.793	814.378	-106.345
450	577.263	817.459	653.730	73.678	505.251	852.729	-98.980
500	628.854	881.003	673.291	103.856	501.330	891.576	-93.140
600	715.454	1003.623	718.219	171.243	495.016	970.252	-84.466
700	784.038	1119.261	767.337	246.347	490.488	1049.846	-78.339
800	839.129	1227.680	818.178	327.602	487.536	1129.962	-73.777
900	884.095	1329.198	869.380	413.836	485.955	1210.357	-70.246
1000	921.296	1424.332	920.169	504.163	485.555	1290.878	-67.427
1100	952.402	1513.642	970.103	597.893	486.114	1371.400	-65.121
1200	978.634	1597.669	1018.934	694.481	487.470	1451.816	-63.195
1300	1000.910	1676.904	1066.529	793.488	489.418	1532.106	-61.560
1400	1019.944	1751.795	1112.827	894.555	491.810	1612.233	-60.152
1500	1036.300	1822.735	1157.810	997.388	494.550	1692.178	-58.926
1600	1050.430	1890.078	1201.490	1101.741	497.494	1771.923	-57.846
1700	1062.696	1954.137	1243.895	1207.411	500.559	1851.452	-56.887
1800	1073.395	2015.189	1285.062	1314.228	503.659	1930.871	-56.031
1900	1082.771	2073.481	1325.035	1422.046	506.760	2010.059	-55.259
2000	1091.022	2129.234	1363.862	1530.745	509.798	2089.114	-54.561
2100	1098.315	2182.645	1401.589	1640.219	512.688	2168.005	-53.925
2200	1104.785	2233.891	1438.264	1750.380	515.429	2246.765	-53.344
2300	1110.549	2283.130	1473.934	1861.152	518.012	2325.402	-52.810
2400	1115.700	2330.506	1508.643	1972.470	520.360	2403.878	-52.318
2500	1120.322	2376.146	1542.436	2084.275	522.485	2482.387	-51.866
2600	1124.480	2420.168	1575.354	2196.519	524.347	2560.687	-51.444
2700	1128.235	2462.678	1607.435	2309.157	525.950	2638.999	-51.053
2800	1131.634	2503.772	1638.717	2422.154	527.265	2717.282	-50.690
2900	1134.721	2543.537	1669.236	2535.474	528.259	2795.464	-50.351
3000	1137.531	2582.054	1699.025	2649.089	528.981	2873.646	-50.034
3100	1140.097	2619.396	1728.115	2762.972	529.344	2951.725	-49.735
3200	1142.444	2655.630	1756.536	2877.101	529.395	3029.878	-49.457
3300	1144.598	2690.819	1784.317	2991.454	529.113	3108.077	-49.196
3400	1146.577	2725.018	1811.484	3106.014	528.467	3186.196	-48.949
3500	1148.400	2758.281	1838.063	3220.765	527.462	3264.318	-48.716
3600	1150.083	2790.656	1864.076	3335.690	526.122	3342.570	-48.498
3700	1151.640	2822.189	1889.547	3450.777	524.413	3420.884	-48.293
3800	1153.082	2852.921	1914.496	3566.014	522.305	3499.181	-48.099
3900	1154.421	2882.890	1938.944	3681.390	519.844	3577.483	-47.914
4000	1155.666	2912.133	1962.910	3796.895	517.012	3656.006	-47.742
4100	1156.825	2940.684	1986.411	3912.520	513.768	3734.522	-47.577
4200	1157.907	2968.574	2009.465	4028.258	510.144	3813.112	-47.422
4300	1158.917	2995.832	2032.088	4144.099	506.124	3891.694	-47.274
4400	1159.862	3022.486	2054.295	4260.039	501.718	3970.476	-47.135
4500	1160.748	3048.561	2076.101	4376.070	496.942	4049.425	-47.004
4600	1161.578	3074.083	2097.520	4492.187	491.739	4128.492	-46.880
4700	1162.359	3099.072	2118.565	4608.384	486.124	4207.551	-46.761
4800	1163.092	3123.552	2139.248	4724.657	480.150	4286.850	-46.649
4900	1163.783	3147.541	2159.582	4841.001	473.734	4366.128	-46.543
5000	1164.434	3171.059	2179.577	4957.412	466.980	4445.750	-46.443

3.440. Naphtho[2,3-s]picene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-66-5
Point Group: C_2

Length: 16.01 Å
Width: 12.92 Å
Breadth: 4.901 Å
L/B Ratio: 1.239

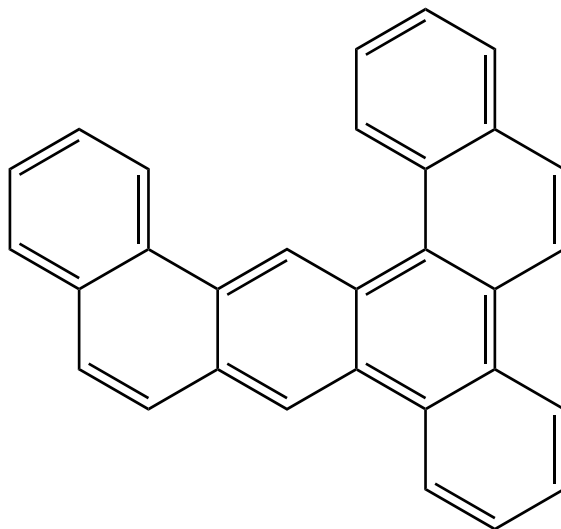
Cartesian coordinates:

C	-0.6618	-5.3649	-0.2631	C	-4.9412	2.1731	-0.1764	H	2.3251	-4.1812	0.9126
C	0.6572	-5.3654	0.2633	C	-5.7126	1.0865	0.1405	H	-2.3287	-4.1792	-0.9124
C	1.3057	-4.1906	0.5107	C	-5.0880	-0.1312	0.4729	H	2.3709	-1.7435	0.7364
C	-1.3092	-4.1895	-0.5109	C	-3.7229	-0.2513	0.4220	H	-2.3719	-1.7413	-0.7377
C	-0.6632	-2.9459	-0.2433	C	0.7243	1.9361	0.0728	H	-0.7965	4.1009	-0.3486
C	0.6610	-2.9464	0.2425	C	1.4499	0.7483	0.0624	H	-3.2516	4.1924	-0.6032
C	1.3245	-1.7168	0.3991	C	2.7476	3.2418	0.3926	H	-5.4046	3.1399	-0.4050
C	-1.3257	-1.7156	-0.3996	C	1.3962	3.1801	0.2697	H	-6.8047	1.1580	0.1574
C	-0.7077	-0.5055	-0.1152	C	3.5286	2.0681	0.1972	H	-5.7047	-0.9824	0.7804
C	0.7076	-0.5060	0.1149	C	2.8910	0.8289	-0.0302	H	-3.2676	-1.2083	0.7110
C	-1.4492	0.7493	-0.0624	C	3.7234	-0.2534	-0.4212	H	3.2540	4.1908	0.6026
C	-0.7229	1.9366	-0.0732	C	5.0886	-0.1338	-0.4721	H	0.7990	4.1005	0.3474
C	-1.3942	3.1808	-0.2705	C	5.7136	1.0837	-0.1399	H	3.2679	-1.2104	-0.7099
C	-2.7456	3.2432	-0.3929	C	4.9427	2.1707	0.1766	H	5.7049	-0.9853	-0.7796
C	-2.8902	0.8306	0.0307	H	-1.1502	-6.3240	-0.4642	H	6.8058	1.1547	-0.1566
C	-3.5273	2.0700	-0.1970	H	1.1447	-6.3249	0.4646	H	5.4064	3.1372	0.4055

Table 3.440: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*s*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.974	557.647	557.647	∞
100	125.754	366.464	859.590	-49.313	587.276	644.140	-336.457
200	246.562	488.672	643.635	-30.993	571.570	707.269	-184.716
250	316.921	551.189	618.865	-16.919	564.200	742.047	-155.039
298.15	385.689	612.902	612.902	0.000	557.647	776.912	-136.109
300	388.301	615.296	612.909	0.716	557.406	778.270	-135.506
350	457.026	680.366	617.891	21.866	551.385	815.571	-121.715
400	520.787	745.619	629.781	46.335	546.181	853.667	-111.475
450	578.545	810.354	646.256	73.844	541.701	892.377	-103.582
500	630.163	874.034	665.860	104.087	537.846	931.575	-97.319
600	716.695	996.889	710.886	171.602	531.660	1010.936	-88.008
700	785.131	1112.708	760.103	246.823	527.249	1091.194	-81.424
800	840.055	1221.262	811.038	328.179	524.398	1171.958	-76.519
900	884.863	1322.879	862.326	414.498	522.901	1252.990	-72.720
1000	921.928	1418.087	913.192	504.895	522.571	1334.138	-69.687
1100	952.922	1507.453	963.196	598.682	523.188	1415.283	-67.205
1200	979.060	1591.520	1012.089	695.317	524.591	1496.315	-65.132
1300	1001.262	1670.787	1059.738	794.363	526.578	1577.218	-63.372
1400	1020.237	1745.701	1106.085	895.463	529.001	1657.956	-61.858
1500	1036.545	1816.660	1151.112	998.322	531.769	1738.509	-60.539
1600	1050.636	1884.018	1194.832	1102.698	534.735	1818.860	-59.378
1700	1062.870	1948.088	1237.272	1208.387	537.819	1898.995	-58.348
1800	1073.544	2009.149	1278.471	1315.220	540.936	1979.019	-57.428
1900	1082.899	2067.449	1318.474	1423.052	544.050	2058.811	-56.599
2000	1091.133	2123.208	1357.327	1531.762	547.100	2138.469	-55.850
2100	1098.412	2176.624	1395.078	1641.247	550.001	2217.961	-55.168
2200	1104.870	2227.874	1431.775	1751.417	552.750	2297.323	-54.544
2300	1110.623	2277.117	1467.466	1862.198	555.341	2376.562	-53.972
2400	1115.767	2324.495	1502.195	1973.522	557.696	2455.640	-53.445
2500	1120.381	2370.138	1536.005	2085.333	559.828	2534.749	-52.960
2600	1124.533	2414.163	1568.939	2197.583	561.695	2613.649	-52.508
2700	1128.282	2456.675	1601.035	2310.226	563.303	2692.562	-52.090
2800	1131.677	2497.770	1632.332	2423.227	564.623	2771.446	-51.701
2900	1134.760	2537.537	1662.864	2536.551	565.621	2850.228	-51.337
3000	1137.567	2576.055	1692.665	2650.170	566.347	2929.009	-50.998
3100	1140.129	2613.398	1721.767	2764.057	566.713	3007.688	-50.678
3200	1142.474	2649.633	1750.199	2878.189	566.767	3086.441	-50.380
3300	1144.625	2684.822	1777.990	2992.545	566.488	3165.241	-50.101
3400	1146.602	2719.022	1805.167	3107.108	565.844	3243.959	-49.836
3500	1148.423	2752.286	1831.755	3221.860	564.842	3322.680	-49.587
3600	1150.105	2784.662	1857.777	3336.788	563.504	3401.532	-49.354
3700	1151.660	2816.195	1883.256	3451.877	561.798	3480.445	-49.134
3800	1153.101	2846.927	1908.213	3567.116	559.692	3559.342	-48.926
3900	1154.438	2876.897	1932.668	3682.494	557.232	3638.243	-48.728
4000	1155.682	2906.141	1956.641	3798.000	554.401	3717.365	-48.543
4100	1156.841	2934.692	1980.149	3913.627	551.159	3796.480	-48.367
4200	1157.921	2962.582	2003.209	4029.366	547.537	3875.670	-48.200
4300	1158.931	2989.841	2025.839	4145.209	543.518	3954.851	-48.041
4400	1159.875	3016.495	2048.052	4261.150	539.114	4034.232	-47.891
4500	1160.760	3042.571	2069.864	4377.182	534.339	4113.780	-47.751
4600	1161.590	3068.092	2091.288	4493.300	529.137	4193.446	-47.617
4700	1162.369	3093.082	2112.338	4609.498	523.523	4273.104	-47.489
4800	1163.103	3117.562	2133.026	4725.772	517.550	4353.002	-47.369
4900	1163.793	3141.551	2153.364	4842.118	511.135	4432.879	-47.254
5000	1164.444	3165.069	2173.363	4958.530	504.382	4513.100	-47.147

3.441. Phenanthro[3,2-g]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-41-6
Point Group: C₁

Length: 15.61 Å
Width: 12.91 Å
Breadth: 5.260 Å
L/B Ratio: 1.209

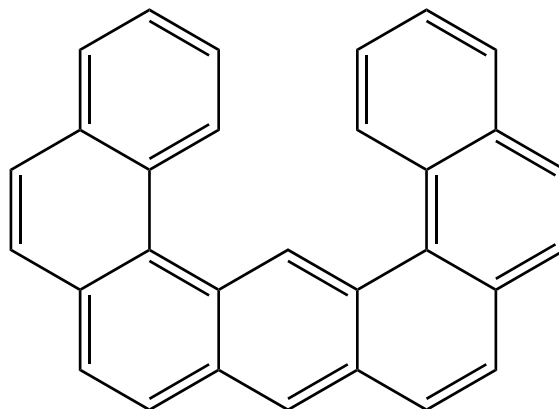
Cartesian coordinates:

C	5.9824	-1.0428	-0.4262	C	-3.9227	-0.8294	-0.6325	H	2.7222	-2.0619	-0.4950
C	5.7961	0.3001	-0.1797	C	-3.8529	-2.1870	-0.6390	H	5.0359	-2.9642	-0.7367
C	3.5989	-1.4014	-0.4088	C	-1.5390	-2.0704	0.1731	H	5.1821	2.8653	0.3070
C	4.8767	-1.8988	-0.5410	C	-2.6700	-2.8359	-0.1859	H	2.8949	3.8071	0.5350
C	3.3852	-0.0307	-0.1594	C	-2.6573	-4.2481	-0.0532	H	0.4692	3.5108	0.4443
C	4.4948	0.8247	-0.0429	C	-1.5727	-4.8857	0.4875	H	1.0745	-1.3708	-0.3020
C	4.2959	2.2268	0.2154	C	-0.4711	-4.1269	0.9303	H	-4.8573	-0.3201	-0.9122
C	3.0510	2.7399	0.3403	C	-0.4569	-2.7647	0.7770	H	-4.7087	-2.7957	-0.9525
C	2.0495	0.5148	-0.0179	C	-2.9546	1.4080	-0.1818	H	-3.5351	-4.8176	-0.3799
C	1.8916	1.8958	0.2185	C	-1.8488	2.2129	0.1309	H	-1.5568	-5.9750	0.5940
C	0.6012	2.4260	0.3013	C	-2.0321	3.5938	0.3304	H	0.3735	-4.6370	1.4055
C	0.9125	-0.2960	-0.1041	C	-3.2799	4.1678	0.1988	H	0.4107	-2.1982	1.1427
C	-0.3781	0.2090	0.0486	C	-4.3782	3.3730	-0.1453	H	-1.1587	4.2133	0.5846
C	-0.5260	1.6146	0.1862	C	-4.2162	2.0154	-0.3321	H	-3.4128	5.2428	0.3573
C	-1.5657	-0.6392	-0.0149	H	6.9933	-1.4494	-0.5336	H	-5.3659	3.8309	-0.2618
C	-2.7927	-0.0342	-0.2828	H	6.6569	0.9723	-0.0885	H	-5.0831	1.3915	-0.5967

Table 3.441: Table of thermodynamic data as a function of temperature for Phenanthro[3,2-g]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-57.075	508.752	508.752	∞
100	126.687	375.132	868.105	-49.297	538.397	594.394	-310.473
200	246.442	497.636	652.339	-30.941	522.728	656.634	-171.492
250	316.368	560.079	627.615	-16.884	515.340	690.965	-144.366
298.15	384.807	621.665	621.665	0.000	508.752	725.404	-127.085
300	387.409	624.053	621.672	0.714	508.509	726.747	-126.535
350	455.909	688.967	626.642	21.814	502.438	763.614	-113.961
400	519.543	754.062	638.503	46.223	497.174	801.283	-104.635
450	577.250	818.647	654.939	73.669	492.631	839.575	-97.453
500	628.869	882.190	674.497	103.847	488.711	878.362	-91.760
600	715.495	1004.816	719.422	171.236	482.399	956.919	-83.306
700	784.072	1120.460	768.540	246.345	477.876	1036.394	-77.335
800	839.141	1228.883	819.380	327.602	474.926	1116.390	-72.891
900	884.081	1330.400	870.582	413.836	473.344	1196.664	-69.451
1000	921.260	1425.532	921.371	504.160	472.942	1277.065	-66.706
1100	952.348	1514.838	971.305	597.886	473.497	1357.468	-64.459
1200	978.566	1598.859	1020.136	694.468	474.847	1437.764	-62.583
1300	1000.834	1678.089	1067.729	793.468	476.788	1517.936	-60.990
1400	1019.863	1752.973	1114.026	894.527	479.171	1597.944	-59.619
1500	1036.217	1823.908	1159.007	997.351	481.903	1677.772	-58.424
1600	1050.345	1891.246	1202.686	1101.696	484.839	1757.399	-57.372
1700	1062.612	1955.300	1245.089	1207.358	487.895	1836.812	-56.437
1800	1073.313	2016.347	1286.254	1314.166	490.988	1916.115	-55.603
1900	1082.692	2074.634	1326.225	1421.977	494.080	1995.188	-54.850
2000	1090.946	2130.383	1365.050	1530.667	497.110	2074.128	-54.170
2100	1098.241	2183.791	1402.775	1640.134	499.993	2152.903	-53.549
2200	1104.715	2235.034	1439.448	1750.288	502.726	2231.549	-52.983
2300	1110.482	2284.270	1475.116	1861.054	505.303	2310.072	-52.462
2400	1115.636	2331.642	1509.824	1972.364	507.644	2388.435	-51.982
2500	1120.261	2377.280	1543.615	2084.163	509.763	2466.830	-51.541
2600	1124.422	2421.300	1576.531	2196.401	511.619	2545.016	-51.129
2700	1128.179	2463.808	1608.610	2309.034	513.216	2623.215	-50.748
2800	1131.582	2504.900	1639.891	2422.025	514.526	2701.386	-50.394
2900	1134.671	2544.663	1670.408	2535.340	515.515	2779.455	-50.062
3000	1137.484	2583.178	1700.195	2648.950	516.232	2857.524	-49.753
3100	1140.051	2620.519	1729.284	2762.829	516.591	2935.491	-49.462
3200	1142.401	2656.751	1757.704	2876.953	516.637	3013.531	-49.190
3300	1144.556	2691.939	1785.483	2991.302	516.350	3091.619	-48.935
3400	1146.537	2726.137	1812.649	3105.858	515.700	3169.626	-48.694
3500	1148.363	2759.399	1839.226	3220.605	514.692	3247.636	-48.467
3600	1150.047	2791.773	1865.238	3335.526	513.348	3325.776	-48.255
3700	1151.605	2823.305	1890.707	3450.610	511.636	3403.979	-48.055
3800	1153.049	2854.035	1915.656	3565.843	509.525	3482.164	-47.865
3900	1154.390	2884.004	1940.102	3681.216	507.060	3560.355	-47.685
4000	1155.636	2913.246	1964.067	3796.718	504.224	3638.767	-47.516
4100	1156.796	2941.797	1987.567	3912.341	500.978	3717.171	-47.356
4200	1157.879	2969.686	2010.620	4028.075	497.351	3795.650	-47.205
4300	1158.890	2996.943	2033.242	4143.914	493.328	3874.121	-47.060
4400	1159.837	3023.596	2055.448	4259.851	488.920	3952.792	-46.925
4500	1160.723	3049.671	2077.254	4375.879	484.141	4031.630	-46.797
4600	1161.555	3075.192	2098.672	4491.994	478.936	4110.586	-46.676
4700	1162.336	3100.181	2119.715	4608.189	473.319	4189.533	-46.560
4800	1163.070	3124.660	2140.398	4724.459	467.342	4268.722	-46.452
4900	1163.762	3148.649	2160.730	4840.801	460.924	4347.890	-46.348
5000	1164.414	3172.167	2180.724	4957.210	454.168	4427.401	-46.252

3.442. Dinaphth[1,2-*a*:2',1'-*j*]anthracene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 68171-26-6
Point Group: C₂

Length: 14.23 Å
Width: 11.54 Å
Breadth: 6.639 Å
L/B Ratio: 1.233

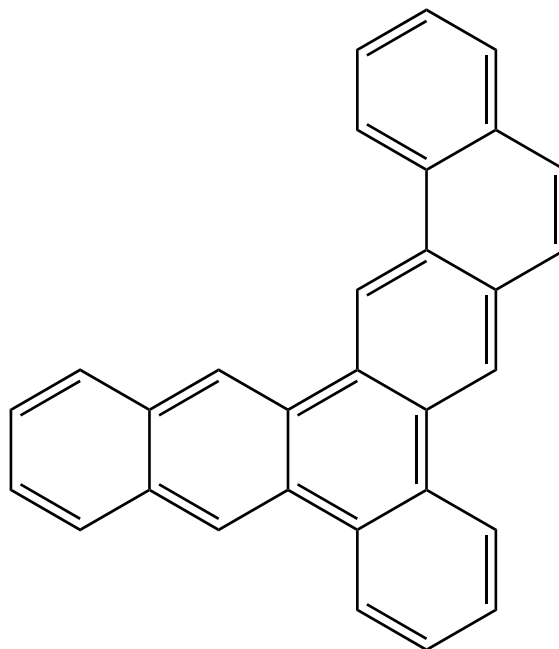
Cartesian coordinates:

C	1.7610	1.6028	1.1244	C	-1.2056	-2.6300	0.1088	H	1.2344	3.4695	2.0365
C	2.7133	0.8519	0.3890	C	0.0039	-3.3164	-0.0021	H	3.3365	4.6058	1.3496
C	3.9457	1.4798	0.1036	C	-2.5137	-0.5307	0.0041	H	5.9557	1.2491	-0.7073
C	4.1505	2.8426	0.4318	C	-3.6339	-1.2606	0.4102	H	5.7191	-1.2030	-1.0449
C	3.1819	3.5530	1.0930	C	-3.5738	-2.6863	0.5699	H	4.5029	-3.2081	-0.8353
C	1.9854	2.9130	1.4657	C	-2.4172	-3.3554	0.3654	H	2.3815	-4.4426	-0.4328
C	2.5150	-0.5250	-0.0046	C	-2.7153	0.8461	-0.3882	H	0.0052	-4.4139	-0.0029
C	3.6370	-1.2518	-0.4110	C	-3.9494	1.4706	-0.1023	H	-0.0005	0.5558	0.0001
C	4.8826	-0.6031	-0.6676	C	-5.0204	0.7207	0.4701	H	-2.3710	-4.4485	0.4278
C	5.0187	0.7328	-0.4692	C	-4.8808	-0.6151	0.6676	H	-4.4951	-3.2192	0.8329
C	1.2313	-1.2106	-0.0091	C	-4.1575	2.8333	-0.4294	H	-5.7159	-1.2171	1.0449
C	1.2118	-2.6271	-0.1119	C	-3.1905	3.5468	-1.0895	H	-5.9587	1.2342	0.7088
C	2.4251	-3.3494	-0.3690	C	-1.9922	2.9102	-1.4624	H	-5.1091	3.3041	-0.1568
C	3.5803	-2.6775	-0.5722	C	-1.7648	1.6000	-1.1227	H	-3.3474	4.5994	-1.3454
C	0.0007	-0.5466	-0.0004	H	5.1005	3.3166	0.1594	H	-1.2424	3.4695	-2.0320
C	-1.2284	-1.2134	0.0075	H	0.8257	1.1245	1.4465	H	-0.8285	1.1242	-1.4455

Table 3.442: Table of thermodynamic data as a function of temperature for Dinaphth[1,2-*a*:2',1'-*j*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.780	532.861	532.861	∞
100	124.133	367.458	858.869	-49.141	562.662	619.426	-323.548
200	245.860	488.781	643.495	-30.943	546.834	682.512	-178.250
250	316.450	551.171	618.761	-16.897	539.436	717.288	-149.866
298.15	385.241	612.805	612.805	0.000	532.861	752.155	-131.772
300	387.852	615.196	612.813	0.715	532.619	753.514	-131.196
350	456.514	680.193	617.789	21.841	526.574	790.822	-118.021
400	520.199	745.372	629.665	46.283	521.343	828.928	-108.245
450	577.902	810.035	646.121	73.761	516.832	867.652	-100.712
500	629.492	873.646	665.704	103.971	512.944	906.868	-94.738
600	716.043	996.379	710.680	171.419	506.691	986.274	-85.861
700	784.554	1112.102	759.847	246.579	502.219	1066.588	-79.588
800	839.570	1220.585	810.733	327.882	499.315	1147.416	-74.917
900	884.469	1322.151	861.976	414.157	497.774	1228.518	-71.300
1000	921.614	1417.321	912.803	504.518	497.409	1309.742	-68.412
1100	952.673	1506.660	962.772	598.277	497.997	1390.964	-66.050
1200	978.865	1590.708	1011.633	694.890	499.378	1472.077	-64.077
1300	1001.109	1669.961	1059.254	793.919	501.348	1553.062	-62.402
1400	1020.116	1744.865	1105.576	895.004	503.757	1633.883	-60.960
1500	1036.451	1815.816	1150.581	997.853	506.514	1714.520	-59.704
1600	1050.561	1883.169	1194.281	1102.220	509.473	1794.956	-58.598
1700	1062.812	1947.235	1236.704	1207.903	512.549	1875.176	-57.616
1800	1073.498	2008.293	1277.887	1314.731	515.661	1955.285	-56.740
1900	1082.863	2066.590	1317.875	1422.559	518.771	2035.162	-55.949
2000	1091.105	2122.348	1356.715	1531.266	521.818	2114.906	-55.235
2100	1098.390	2175.763	1394.454	1640.748	524.716	2194.485	-54.584
2200	1104.853	2227.012	1431.141	1750.917	527.464	2273.933	-53.989
2300	1110.610	2276.254	1466.822	1861.695	530.053	2353.258	-53.443
2400	1115.757	2323.632	1501.541	1973.018	532.407	2432.422	-52.939
2500	1120.373	2369.275	1535.343	2084.829	534.538	2511.618	-52.476
2600	1124.528	2413.299	1568.269	2197.078	536.405	2590.605	-52.045
2700	1128.279	2455.811	1600.358	2309.721	538.012	2669.604	-51.646
2800	1131.675	2496.906	1631.648	2422.722	539.332	2748.574	-51.274
2900	1134.759	2536.672	1662.174	2536.046	540.330	2827.442	-50.927
3000	1137.567	2575.191	1691.969	2649.664	541.055	2906.310	-50.602
3100	1140.130	2612.534	1721.066	2763.551	541.422	2985.075	-50.297
3200	1142.475	2648.769	1749.493	2877.683	541.476	3063.915	-50.012
3300	1144.626	2683.958	1777.280	2992.039	541.196	3142.801	-49.745
3400	1146.604	2718.158	1804.452	3106.602	540.553	3221.605	-49.493
3500	1148.426	2751.422	1831.035	3221.355	539.551	3300.413	-49.255
3600	1150.107	2783.798	1857.053	3336.283	538.214	3379.351	-49.032
3700	1151.663	2815.332	1882.528	3451.372	536.507	3458.351	-48.822
3800	1153.104	2846.064	1907.482	3566.611	534.402	3537.334	-48.623
3900	1154.441	2876.034	1931.934	3681.990	531.943	3616.321	-48.434
4000	1155.685	2905.277	1955.903	3797.497	529.112	3695.530	-48.258
4100	1156.844	2933.829	1979.408	3913.124	525.870	3774.731	-48.090
4200	1157.924	2961.719	2002.466	4028.863	522.248	3854.007	-47.931
4300	1158.934	2988.977	2025.092	4144.706	518.229	3933.274	-47.779
4400	1159.878	3015.632	2047.303	4260.647	513.825	4012.742	-47.636
4500	1160.763	3041.708	2069.112	4376.680	509.051	4092.376	-47.502
4600	1161.593	3067.229	2090.534	4492.798	503.849	4172.128	-47.375
4700	1162.372	3092.219	2111.581	4608.997	498.236	4251.872	-47.253
4800	1163.106	3116.699	2132.267	4725.271	492.263	4331.857	-47.139
4900	1163.796	3140.688	2152.603	4841.617	485.849	4411.821	-47.030
5000	1164.447	3164.207	2172.601	4958.029	479.096	4492.128	-46.928

3.443. Dibenzo[*a,h*]pentaphene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-38-1
Point Group: C_s

Length: 16.08 Å
Width: 13.13 Å
Breadth: 3.888 Å
L/B Ratio: 1.225

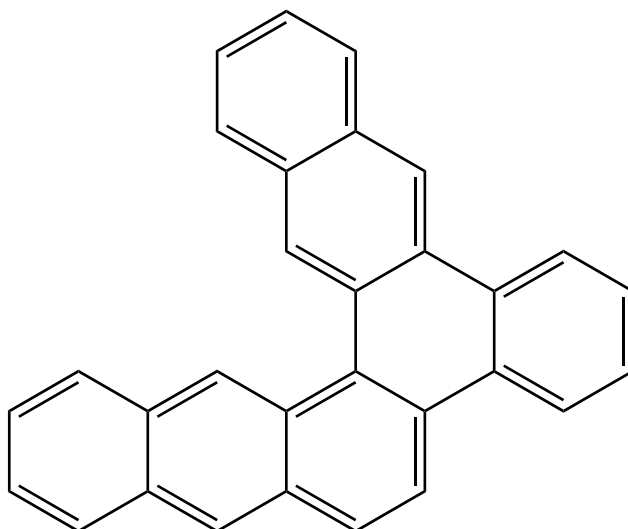
Cartesian coordinates:

C	4.1830	-4.2113	0.0000	C	-0.0459	0.2761	0.0000	H	6.0542	-1.3497	0.0000
C	5.3223	-3.3676	0.0000	C	-0.2031	1.6845	0.0000	H	2.0394	-4.3227	0.0000
C	5.1789	-2.0089	0.0000	C	-1.4829	2.2265	0.0000	H	4.5871	0.6286	0.0000
C	2.9252	-3.6777	0.0000	C	-1.1748	-0.5338	0.0000	H	0.5748	-2.3411	0.0000
C	2.7457	-2.2647	0.0000	C	-2.4681	0.0079	0.0000	H	4.3860	2.3955	0.0000
C	3.8798	-1.4249	0.0000	C	-2.6220	1.4080	0.0000	H	4.1051	4.8648	0.0000
C	3.6998	-0.0249	0.0000	C	-3.9415	1.9809	0.0000	H	1.8212	5.8575	0.0000
C	1.4593	-1.6838	0.0000	C	-5.0400	1.1907	0.0000	H	-0.1759	4.3782	0.0000
C	1.2908	-0.3118	0.0000	C	-3.6443	-0.8363	0.0000	H	-1.6048	3.3218	0.0000
C	2.4370	0.5371	0.0000	C	-4.9187	-0.2425	0.0000	H	-1.0638	-1.6354	0.0000
C	0.9743	2.5470	0.0000	C	-6.0675	-1.0608	0.0000	H	-4.0309	3.0733	0.0000
C	2.2626	1.9868	0.0000	C	-5.9440	-2.4326	0.0000	H	-6.0470	1.6236	0.0000
C	3.3783	2.8387	0.0000	C	-4.6724	-3.0275	0.0000	H	-7.0583	-0.5922	0.0000
C	3.2249	4.2137	0.0000	C	-3.5410	-2.2426	0.0000	H	-6.8361	-3.0674	0.0000
C	1.9456	4.7698	0.0000	H	4.3278	-5.2966	0.0000	H	-4.5866	-4.1189	0.0000
C	0.8357	3.9440	0.0000	H	6.3182	-3.8227	0.0000	H	-2.5362	-2.6925	0.0000

Table 3.443: Table of thermodynamic data as a function of temperature for Dibenzo[*a,h*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-57.749	488.231	488.231	∞
100	129.295	393.127	888.623	-49.550	517.624	571.821	-298.683
200	247.594	516.960	672.008	-31.010	502.137	632.179	-165.105
250	317.044	579.605	647.238	-16.908	494.795	665.539	-139.054
298.15	385.145	641.280	641.280	0.000	488.231	699.035	-122.466
300	387.736	643.670	641.287	0.715	487.989	700.342	-121.938
350	455.978	708.615	646.260	21.824	481.927	736.227	-109.874
400	519.427	773.705	658.125	46.232	476.662	772.914	-100.930
450	577.010	838.269	674.562	73.668	472.109	810.224	-94.046
500	628.551	901.783	694.119	103.832	468.175	848.030	-88.591
600	715.115	1024.344	739.034	171.186	461.828	924.632	-80.495
700	783.701	1139.930	788.135	246.256	457.266	1002.157	-74.780
800	838.807	1248.304	838.957	327.478	454.281	1080.207	-70.529
900	883.792	1349.785	890.139	413.681	452.669	1158.542	-67.239
1000	921.014	1444.888	940.910	503.979	452.240	1237.005	-64.613
1100	952.141	1534.173	990.826	597.682	452.772	1315.474	-62.465
1200	978.392	1618.178	1039.640	694.245	454.103	1393.838	-60.671
1300	1000.687	1697.395	1087.219	793.228	456.028	1472.078	-59.148
1400	1019.739	1772.269	1133.502	894.274	458.397	1550.156	-57.836
1500	1036.111	1843.196	1178.472	997.087	461.118	1628.055	-56.693
1600	1050.254	1910.528	1222.139	1101.422	464.044	1705.754	-55.686
1700	1062.534	1974.576	1264.531	1207.076	467.092	1783.239	-54.791
1800	1073.245	2035.619	1305.687	1313.877	470.177	1860.614	-53.993
1900	1082.632	2093.903	1345.650	1421.681	473.263	1937.760	-53.272
2000	1090.894	2149.649	1384.467	1530.366	476.288	2014.773	-52.619
2100	1098.195	2203.055	1422.184	1639.827	479.166	2091.622	-52.025
2200	1104.674	2254.295	1458.851	1749.977	481.894	2168.342	-51.482
2300	1110.445	2303.530	1494.513	1860.739	484.467	2244.938	-50.983
2400	1115.603	2350.901	1529.215	1972.046	486.805	2321.375	-50.522
2500	1120.231	2396.537	1563.001	2083.842	488.921	2397.845	-50.099
2600	1124.395	2440.556	1595.911	2196.077	490.774	2474.105	-49.704
2700	1128.155	2483.063	1627.986	2308.707	492.368	2550.379	-49.339
2800	1131.559	2524.154	1659.262	2421.696	493.676	2626.624	-48.999
2900	1134.650	2563.916	1689.776	2535.009	494.663	2702.768	-48.681
3000	1137.465	2602.431	1719.559	2648.616	495.378	2778.912	-48.384
3100	1140.034	2639.771	1748.644	2762.493	495.734	2854.953	-48.105
3200	1142.385	2676.003	1777.061	2876.616	495.779	2931.069	-47.844
3300	1144.541	2711.190	1804.837	2990.964	495.491	3007.231	-47.600
3400	1146.523	2745.387	1832.000	3105.518	494.840	3083.313	-47.368
3500	1148.349	2778.649	1858.574	3220.263	493.829	3159.398	-47.150
3600	1150.035	2811.023	1884.583	3335.184	492.485	3235.613	-46.947
3700	1151.594	2842.554	1910.050	3450.266	490.771	3311.891	-46.755
3800	1153.039	2873.285	1934.996	3565.499	488.659	3388.151	-46.572
3900	1154.379	2903.253	1959.440	3680.870	486.194	3464.417	-46.400
4000	1155.626	2932.495	1983.402	3796.371	483.357	3540.904	-46.239
4100	1156.787	2961.045	2006.901	3911.993	480.109	3617.383	-46.085
4200	1157.871	2988.934	2029.952	4027.726	476.481	3693.938	-45.940
4300	1158.882	3016.191	2052.572	4143.565	472.458	3770.483	-45.801
4400	1159.829	3042.844	2074.776	4259.501	468.049	3847.230	-45.671
4500	1160.716	3068.919	2096.579	4375.528	463.269	3924.143	-45.549
4600	1161.548	3094.440	2117.996	4491.642	458.063	4001.174	-45.434
4700	1162.329	3119.428	2139.038	4607.836	452.445	4078.197	-45.323
4800	1163.064	3143.907	2159.718	4724.106	446.468	4155.461	-45.220
4900	1163.756	3167.896	2180.050	4840.448	440.050	4232.704	-45.120
5000	1164.408	3191.414	2200.042	4956.856	433.293	4310.290	-45.028

3.444. Benzo[*b*]naphtho[2,3-*g*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-65-4
Point Group: C₁

Length: 15.88 Å
Width: 12.85 Å
Breadth: 5.382 Å
L/B Ratio: 1.236

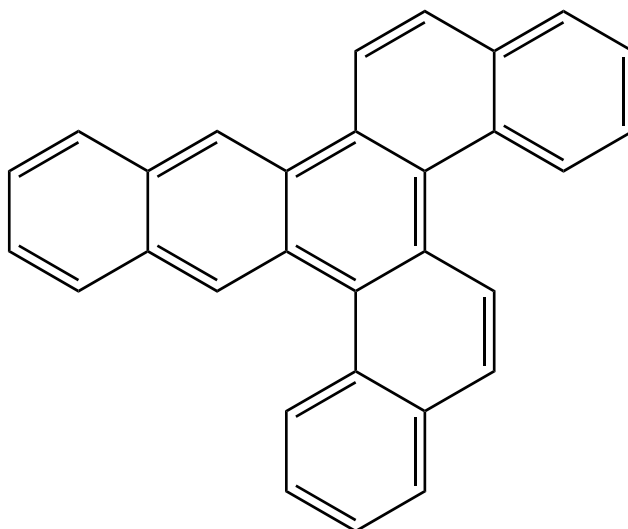
Cartesian coordinates:

C	5.4838	-1.8350	-0.8362	C	-3.1787	-1.0673	-0.2767	H	6.3273	1.2310	0.4297
C	6.2904	-0.7577	-0.3710	C	-0.5298	-1.5432	0.4208	H	3.4986	-2.5578	-1.1953
C	5.7167	0.3943	0.0724	C	-1.4286	-2.6252	0.3477	H	4.2868	2.5727	0.8021
C	4.1264	-1.7337	-0.8378	C	-2.7658	-2.3905	-0.0375	H	1.4976	-1.2768	-0.7029
C	3.4881	-0.5407	-0.3692	C	-3.6671	-3.4906	-0.1429	H	2.3163	3.9238	1.1122
C	4.2927	0.5363	0.0787	C	-3.2408	-4.7560	0.1392	H	-0.1211	4.2456	0.7954
C	3.6717	1.7196	0.4894	C	-1.9001	-4.9915	0.5424	H	-4.2323	-0.8713	-0.5334
C	2.0933	-0.4249	-0.3434	C	-1.0151	-3.9578	0.6459	H	0.5049	-1.7595	0.7251
C	1.4576	0.7286	0.1189	C	-2.7791	1.3601	-0.2822	H	-4.7006	-3.2970	-0.4510
C	2.2823	1.8333	0.4843	C	-1.9169	2.4247	0.0215	H	-3.9256	-5.6067	0.0607
C	1.6753	3.0953	0.7897	C	-2.4266	3.7368	0.0077	H	-1.5895	-6.0169	0.7682
C	0.3419	3.2608	0.6321	C	-3.7421	3.9851	-0.3290	H	0.0213	-4.1309	0.9572
C	0.0127	0.8823	0.1683	C	-4.5903	2.9250	-0.6632	H	-1.7602	4.5737	0.2645
C	-0.5091	2.1622	0.2788	C	-4.1137	1.6299	-0.6352	H	-4.1235	5.0113	-0.3391
C	-0.9152	-0.2461	0.1174	H	5.9775	-2.7452	-1.1921	H	-5.6303	3.1247	-0.9406
C	-2.2936	-0.0063	-0.1723	H	7.3790	-0.8746	-0.3788	H	-4.7781	0.7874	-0.8803

Table 3.444: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[2,3-*g*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.250	528.808	528.808	∞
100	126.817	376.336	870.848	-49.451	558.299	614.175	-320.806
200	247.280	499.172	654.384	-31.042	542.682	676.281	-176.623
250	317.426	561.827	629.579	-16.938	535.342	710.530	-148.454
298.15	385.979	623.610	623.610	0.000	528.808	744.880	-130.497
300	388.583	626.006	623.618	0.716	528.567	746.219	-129.926
350	457.106	691.104	628.602	21.876	522.555	782.984	-116.852
400	520.703	756.356	640.496	46.344	517.351	820.542	-107.150
450	578.344	821.075	656.972	73.846	512.864	858.716	-99.675
500	629.885	884.729	676.576	104.077	508.997	897.379	-93.747
600	716.364	1007.527	721.593	171.560	502.779	975.673	-84.938
700	784.822	1123.296	770.797	246.749	498.336	1054.870	-78.714
800	839.800	1231.812	821.716	328.077	495.457	1134.577	-74.079
900	884.668	1333.403	872.988	414.373	493.937	1214.555	-70.489
1000	921.789	1428.593	923.840	504.753	493.591	1294.652	-67.624
1100	952.828	1517.947	973.830	598.529	494.196	1374.747	-65.280
1200	979.004	1602.008	1022.711	695.157	495.592	1454.730	-63.321
1300	1001.234	1681.272	1070.350	794.199	497.575	1534.585	-61.659
1400	1020.230	1756.185	1116.687	895.296	499.996	1614.273	-60.228
1500	1036.554	1827.144	1161.707	998.156	502.764	1693.779	-58.981
1600	1050.655	1894.503	1205.419	1102.533	505.732	1773.081	-57.884
1700	1062.898	1958.574	1247.854	1208.225	508.818	1852.168	-56.909
1800	1073.578	2019.637	1289.048	1315.061	511.937	1931.142	-56.039
1900	1082.936	2077.938	1329.046	1422.896	515.055	2009.885	-55.254
2000	1091.172	2133.700	1367.894	1531.610	518.109	2088.494	-54.545
2100	1098.452	2187.118	1405.642	1641.099	521.014	2166.938	-53.899
2200	1104.911	2238.370	1442.336	1751.273	523.767	2245.250	-53.308
2300	1110.664	2287.614	1478.024	1862.058	526.363	2323.439	-52.766
2400	1115.807	2334.994	1512.750	1973.386	528.722	2401.467	-52.265
2500	1120.420	2380.639	1546.559	2085.201	530.857	2479.527	-51.806
2600	1124.572	2424.665	1579.490	2197.454	532.728	2557.377	-51.377
2700	1128.320	2467.178	1611.585	2310.102	534.340	2635.239	-50.981
2800	1131.713	2508.275	1642.880	2423.107	535.664	2713.073	-50.612
2900	1134.795	2548.043	1673.410	2536.434	536.665	2790.804	-50.267
3000	1137.601	2586.562	1703.210	2650.056	537.394	2868.535	-49.945
3100	1140.162	2623.906	1732.311	2763.946	537.764	2946.163	-49.641
3200	1142.505	2660.142	1760.742	2878.082	537.822	3023.865	-49.359
3300	1144.655	2695.333	1788.532	2992.441	537.545	3101.613	-49.093
3400	1146.631	2729.534	1815.708	3107.007	536.905	3179.280	-48.843
3500	1148.451	2762.798	1842.295	3221.762	535.905	3256.951	-48.606
3600	1150.132	2795.175	1868.316	3336.692	534.570	3334.751	-48.385
3700	1151.686	2826.709	1893.794	3451.784	532.866	3412.613	-48.176
3800	1153.126	2857.442	1918.751	3567.026	530.763	3490.458	-47.979
3900	1154.463	2887.412	1943.206	3682.406	528.306	3568.308	-47.791
4000	1155.705	2916.657	1967.178	3797.915	525.477	3646.379	-47.616
4100	1156.863	2945.208	1990.685	3913.544	522.237	3724.442	-47.449
4200	1157.943	2973.099	2013.745	4029.285	518.617	3802.580	-47.291
4300	1158.951	3000.358	2036.374	4145.130	514.600	3880.709	-47.140
4400	1159.895	3027.013	2058.587	4261.073	510.198	3959.038	-46.999
4500	1160.779	3053.089	2080.398	4377.107	505.425	4037.535	-46.866
4600	1161.608	3078.611	2101.822	4493.227	500.225	4116.149	-46.739
4700	1162.387	3103.601	2122.872	4609.427	494.613	4194.755	-46.619
4800	1163.120	3128.081	2143.559	4725.703	488.642	4273.601	-46.505
4900	1163.810	3152.071	2163.897	4842.050	482.229	4352.427	-46.396
5000	1164.460	3175.589	2183.897	4958.464	475.478	4431.596	-46.296

3.445. Benzo[*b*]naphtho[2,1-*p*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-67-6
Point Group: C₁

Length: 16.07 Å
Width: 12.97 Å
Breadth: 5.779 Å
L/B Ratio: 1.240

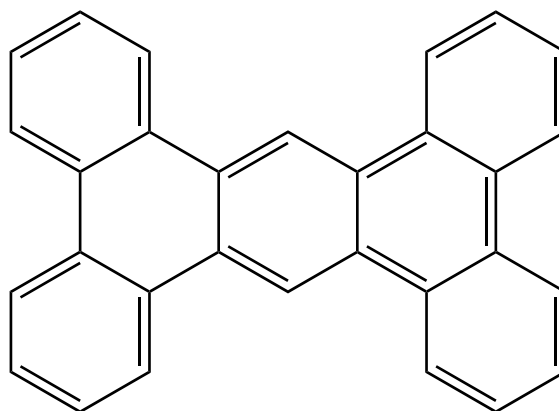
Cartesian coordinates:

C	5.6991	1.7408	-0.0750	C	-4.9164	2.4028	0.2279	H	3.4573	4.3248	-0.0857
C	5.1979	3.0699	-0.0860	C	-5.8282	1.3898	0.3630	H	5.2231	-0.3506	-0.0432
C	3.8540	3.3035	-0.0753	C	-5.3827	0.0534	0.3803	H	1.1661	3.4446	-0.0922
C	4.8448	0.6778	-0.0508	C	-4.0530	-0.2397	0.2209	H	2.9485	-1.2014	-0.0170
C	3.4329	0.8901	-0.0343	C	0.2069	-1.0983	-0.0422	H	-0.5405	3.7473	0.0576
C	2.9359	2.2110	-0.0513	C	-1.1241	-0.8154	-0.3570	H	-2.9683	4.2170	0.0769
C	1.5456	2.4113	-0.0572	C	-1.9145	-1.8397	-0.9589	H	-5.2398	3.4501	0.2346
C	2.5278	-0.1851	-0.0061	C	-1.4696	-3.1212	-1.0534	H	-6.8959	1.6058	0.4703
C	1.1526	0.0082	0.0226	C	0.5854	-2.4837	0.1130	H	-6.1108	-0.7513	0.5270
C	0.6561	1.3460	-0.0269	C	-0.2423	-3.4879	-0.4314	H	-3.7350	-1.2909	0.2441
C	-1.6705	0.5179	-0.1391	C	0.1197	-4.8538	-0.3281	H	-2.8945	-1.5712	-1.3765
C	-0.7794	1.5821	-0.0437	C	1.2446	-5.2221	0.3629	H	-2.0585	-3.8890	-1.5677
C	-1.2657	2.9204	0.0314	C	2.0337	-4.2354	0.9855	H	-0.5217	-5.6087	-0.7971
C	-2.5983	3.1855	0.0547	C	1.7142	-2.9070	0.8615	H	1.5292	-6.2756	0.4497
C	-3.0806	0.7786	0.0329	H	6.7830	1.5858	-0.0863	H	2.9042	-4.5399	1.5761
C	-3.5345	2.1142	0.0904	H	5.9093	3.9020	-0.1043	H	2.3372	-2.1542	1.3638

Table 3.445: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[2,1-*p*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.385	547.953	547.953	∞
100	127.161	378.393	873.757	-49.536	577.359	633.030	-330.654
200	247.676	501.478	656.936	-31.092	561.777	694.915	-181.490
250	317.926	564.232	632.092	-16.965	554.460	729.047	-152.323
298.15	386.599	626.113	626.113	0.000	547.953	763.279	-133.721
300	389.207	628.513	626.121	0.718	547.714	764.613	-133.128
350	457.842	693.716	631.113	21.911	541.736	801.250	-119.578
400	521.521	759.072	643.026	46.419	536.571	838.675	-109.517
450	579.206	823.890	659.528	73.963	532.125	876.710	-101.764
500	630.760	887.636	679.163	104.237	528.302	915.230	-95.611
600	717.192	1010.590	724.247	171.806	522.170	993.226	-86.466
700	785.557	1126.480	773.518	247.074	517.805	1072.110	-80.000
800	840.429	1235.088	824.501	328.469	514.994	1151.494	-75.183
900	885.199	1336.747	875.831	414.824	513.533	1231.141	-71.452
1000	922.232	1431.988	926.736	505.252	513.235	1310.901	-68.473
1100	953.199	1521.381	976.774	599.068	513.880	1390.654	-66.035
1200	979.315	1605.472	1025.696	695.730	515.310	1470.292	-63.999
1300	1001.496	1684.758	1073.373	794.800	517.321	1549.799	-62.270
1400	1020.452	1759.689	1119.744	895.922	519.767	1629.139	-60.783
1500	1036.743	1830.662	1164.794	998.802	522.555	1708.293	-59.487
1600	1050.818	1898.032	1208.534	1103.197	525.541	1787.243	-58.346
1700	1063.039	1962.113	1250.993	1208.904	528.642	1865.976	-57.333
1800	1073.701	2023.183	1292.209	1315.753	531.775	1944.596	-56.430
1900	1083.044	2081.491	1332.228	1423.600	534.904	2022.984	-55.615
2000	1091.268	2137.257	1371.095	1532.324	537.968	2101.238	-54.878
2100	1098.537	2190.680	1408.860	1641.822	540.882	2179.325	-54.207
2200	1104.987	2241.936	1445.570	1752.005	543.643	2257.281	-53.594
2300	1110.732	2291.183	1481.272	1862.796	546.246	2335.113	-53.031
2400	1115.868	2338.566	1516.012	1974.131	548.612	2412.784	-52.512
2500	1120.476	2384.213	1549.833	2085.952	550.753	2490.487	-52.035
2600	1124.622	2428.241	1582.776	2198.210	552.629	2567.979	-51.590
2700	1128.366	2470.756	1614.881	2310.863	554.246	2645.484	-51.179
2800	1131.756	2511.855	1646.186	2423.872	555.574	2722.959	-50.796
2900	1134.834	2551.624	1676.726	2537.204	556.580	2800.333	-50.438
3000	1137.637	2590.145	1706.535	2650.829	557.312	2877.705	-50.104
3100	1140.195	2627.490	1735.644	2764.723	557.686	2954.975	-49.790
3200	1142.537	2663.727	1764.083	2878.861	557.746	3032.319	-49.497
3300	1144.684	2698.918	1791.881	2993.224	557.473	3109.708	-49.222
3400	1146.658	2733.120	1819.064	3107.792	556.835	3187.017	-48.962
3500	1148.477	2766.386	1845.657	3222.550	555.838	3264.329	-48.716
3600	1150.155	2798.763	1871.684	3337.483	554.506	3341.770	-48.487
3700	1151.708	2830.298	1897.169	3452.577	552.804	3419.274	-48.270
3800	1153.147	2861.031	1922.131	3567.821	550.703	3496.760	-48.065
3900	1154.482	2891.002	1946.591	3683.203	548.248	3574.250	-47.871
4000	1155.724	2920.247	1970.568	3798.714	545.421	3651.962	-47.689
4100	1156.881	2948.799	1994.081	3914.345	542.183	3729.667	-47.516
4200	1157.959	2976.690	2017.145	4030.088	538.565	3807.445	-47.352
4300	1158.967	3003.949	2039.779	4145.935	534.550	3885.215	-47.195
4400	1159.910	3030.604	2061.996	4261.879	530.149	3963.186	-47.048
4500	1160.793	3056.681	2083.811	4377.915	525.378	4041.323	-46.909
4600	1161.622	3082.203	2105.239	4494.036	520.179	4119.578	-46.778
4700	1162.400	3107.194	2126.292	4610.237	514.568	4197.824	-46.653
4800	1163.132	3131.674	2146.983	4726.514	508.598	4276.311	-46.535
4900	1163.821	3155.664	2167.325	4842.862	502.186	4354.778	-46.422
5000	1164.471	3179.183	2187.327	4959.277	495.436	4433.587	-46.316

3.446. Phenanthro[9,10-*b*]triphenylene



Other names: Tetrabenz[*a,c,h,j*]anthracene

Formula: C₃₀H₁₈

Mass: 378.464 g/mol

CAS Number: 215-11-2

Point Group: D_{2h}

Length: 14.11 Å

Width: 11.65 Å

Breadth: 3.885 Å

L/B Ratio: 1.211

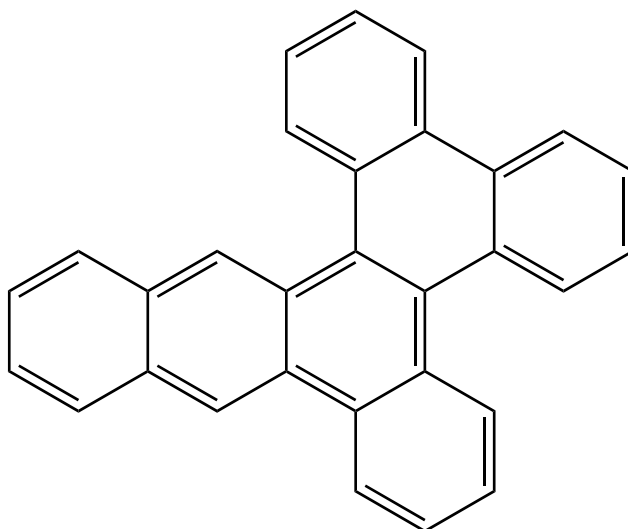
Cartesian coordinates:

C	4.9111	-2.8234	0.0000	C	-1.2191	-0.7068	0.0000	H	1.5489	-3.3791	0.0000
C	4.9069	-1.4422	0.0000	C	-1.2207	0.7039	0.0000	H	3.7062	-4.6193	0.0000
C	2.5057	-2.8345	0.0000	C	-2.4798	-1.4345	0.0000	H	5.8532	0.8972	0.0000
C	3.7020	-3.5246	0.0000	C	-3.6967	-0.7323	0.0000	H	5.8511	3.3848	0.0000
C	2.4832	-1.4286	0.0000	C	-4.9035	-1.4538	0.0000	H	3.6953	4.6281	0.0000
C	3.6984	-0.7235	0.0000	C	-4.9043	-2.8350	0.0000	H	1.5410	3.3828	0.0000
C	2.4798	1.4345	0.0000	C	-3.6936	-3.5334	0.0000	H	-0.0029	2.4908	0.0000
C	3.6967	0.7323	0.0000	C	-2.4989	-2.8404	0.0000	H	0.0030	-2.4907	0.0000
C	4.9035	1.4538	0.0000	C	-3.6984	0.7235	0.0000	H	-5.8532	-0.8972	0.0000
C	4.9044	2.8350	0.0000	C	-2.4832	1.4287	0.0000	H	-5.8511	-3.3848	0.0000
C	3.6937	3.5333	0.0000	C	-2.5057	2.8345	0.0000	H	-3.6952	-4.6281	0.0000
C	2.4990	2.8404	0.0000	C	-3.7021	3.5246	0.0000	H	-1.5409	-3.3828	0.0000
C	1.2208	-0.7039	0.0000	C	-4.9112	2.8233	0.0000	H	-1.5490	3.3792	0.0000
C	1.2191	0.7068	0.0000	C	-4.9070	1.4421	0.0000	H	-3.7064	4.6193	0.0000
C	-0.0016	1.3838	0.0000	H	5.8591	-3.3709	0.0000	H	-5.8592	3.3708	0.0000
C	0.0017	-1.3837	0.0000	H	5.8553	-0.8833	0.0000	H	-5.8553	0.8832	0.0000

Table 3.446: Table of thermodynamic data as a function of temperature for Phenanthro[9,10-*b*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.702	487.983	487.983	∞
100	130.243	373.046	868.807	-49.576	517.349	573.554	-299.588
200	247.686	497.293	652.200	-30.981	501.917	635.892	-166.075
250	316.721	559.912	627.456	-16.886	494.569	670.236	-140.035
298.15	384.579	621.507	621.507	0.000	487.983	704.682	-123.455
300	387.163	623.894	621.514	0.714	487.739	706.025	-122.927
350	455.302	688.740	626.480	21.791	481.646	742.901	-110.870
400	518.738	753.740	638.327	46.165	476.347	780.584	-101.932
450	576.349	818.224	654.741	73.567	471.760	818.895	-95.053
500	627.930	881.670	674.272	103.699	467.794	857.705	-89.602
600	714.561	1004.124	719.133	170.995	461.388	936.324	-81.513
700	783.179	1119.627	768.182	246.011	456.773	1015.875	-75.804
800	838.295	1227.933	818.956	327.182	453.736	1095.959	-71.557
900	883.283	1329.354	870.094	413.334	452.072	1176.334	-68.271
1000	920.508	1424.403	920.823	503.580	451.593	1256.843	-65.649
1100	951.642	1513.640	970.701	597.233	452.074	1337.363	-63.505
1200	977.905	1597.602	1019.479	693.747	453.356	1417.782	-61.713
1300	1000.216	1676.781	1067.025	792.682	455.233	1498.082	-60.192
1400	1019.288	1751.621	1113.276	893.682	457.557	1578.223	-58.883
1500	1035.681	1822.517	1158.217	996.451	460.233	1658.188	-57.742
1600	1049.847	1889.822	1201.857	1100.744	463.118	1737.956	-56.737
1700	1062.149	1953.846	1244.224	1206.358	466.126	1817.513	-55.844
1800	1072.882	2014.868	1285.355	1313.122	469.173	1896.963	-55.047
1900	1082.290	2073.133	1325.296	1420.890	472.224	1976.185	-54.328
2000	1090.572	2128.862	1364.091	1529.542	475.216	2055.276	-53.677
2100	1097.892	2182.252	1401.789	1638.973	478.062	2134.204	-53.084
2200	1104.389	2233.479	1438.436	1749.093	480.762	2213.005	-52.542
2300	1110.177	2282.701	1474.081	1859.827	483.307	2291.684	-52.045
2400	1115.351	2330.061	1508.766	1971.108	485.619	2370.204	-51.585
2500	1119.993	2375.688	1542.536	2082.879	487.710	2448.758	-51.163
2600	1124.171	2419.697	1575.432	2195.091	489.540	2527.104	-50.769
2700	1127.943	2462.196	1607.492	2307.700	491.113	2605.464	-50.405
2800	1131.359	2503.279	1638.755	2420.668	492.399	2683.796	-50.066
2900	1134.461	2543.035	1669.255	2533.961	493.367	2762.028	-49.748
3000	1137.285	2581.543	1699.026	2647.551	494.063	2840.260	-49.452
3100	1139.864	2618.877	1728.100	2761.410	494.403	2918.390	-49.174
3200	1142.224	2655.104	1756.506	2875.516	494.431	2996.596	-48.913
3300	1144.388	2690.286	1784.272	2989.848	494.127	3074.848	-48.670
3400	1146.378	2724.480	1811.424	3104.388	493.461	3153.020	-48.439
3500	1148.211	2757.737	1837.989	3219.119	492.436	3231.197	-48.222
3600	1149.903	2790.107	1863.989	3334.026	491.078	3309.503	-48.019
3700	1151.468	2821.635	1889.447	3449.095	489.352	3387.873	-47.827
3800	1152.918	2852.362	1914.384	3564.315	487.227	3466.225	-47.646
3900	1154.265	2882.327	1938.821	3679.675	484.750	3544.583	-47.473
4000	1155.517	2911.567	1962.775	3795.165	481.902	3623.163	-47.313
4100	1156.682	2940.114	1986.266	3910.776	478.643	3701.736	-47.160
4200	1157.770	2968.000	2009.310	4026.499	475.006	3780.383	-47.015
4300	1158.786	2995.255	2031.923	4142.327	470.972	3859.022	-46.877
4400	1159.737	3021.906	2054.121	4258.254	466.554	3937.862	-46.747
4500	1160.627	3047.979	2075.918	4374.273	461.765	4016.869	-46.626
4600	1161.463	3073.498	2097.328	4490.378	456.550	4095.994	-46.511
4700	1162.247	3098.485	2118.365	4606.564	450.924	4175.112	-46.400
4800	1162.985	3122.962	2139.040	4722.826	444.939	4254.470	-46.297
4900	1163.680	3146.949	2159.365	4839.159	438.513	4333.808	-46.198
5000	1164.335	3170.465	2179.353	4955.560	431.749	4413.489	-46.106

3.447. Tribenzo[*b,g,p*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-77-8
Point Group: C₁

Length: 15.91 Å
Width: 12.80 Å
Breadth: 4.919 Å
L/B Ratio: 1.243

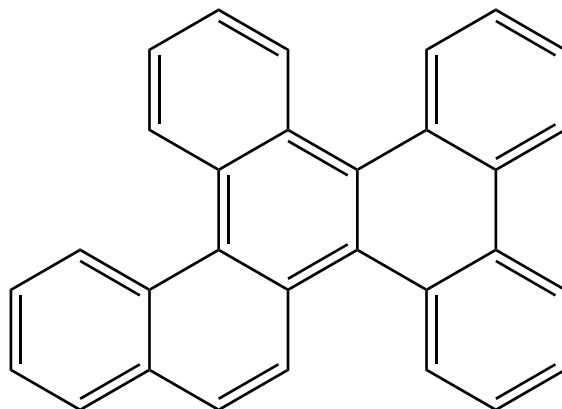
Cartesian coordinates:

C	-5.6378	-1.7490	-0.4266	C	0.3896	-0.3997	0.0213	H	-5.6007	1.4636	0.7470
C	-6.1147	-0.5064	0.0665	C	1.2554	0.6804	-0.0165	H	-3.9238	-2.9196	-0.9704
C	-5.2428	0.4986	0.3712	C	3.1967	-0.8414	-0.1723	H	-3.2825	2.3418	0.7089
C	-4.2996	-1.9625	-0.5915	C	2.6918	0.4528	0.0524	H	-1.6352	-2.1308	-0.7358
C	-3.3631	-0.9365	-0.2676	C	3.6257	1.4643	0.3688	H	-2.1687	3.7294	0.6341
C	-3.8405	0.3069	0.1997	C	4.9835	1.2418	0.3056	H	-0.7121	5.6749	0.0827
C	-2.9148	1.3409	0.4314	C	5.4735	-0.0141	-0.0752	H	1.5773	5.2718	-0.8178
C	-1.9740	-1.1471	-0.3800	C	4.5879	-1.0445	-0.2919	H	2.4863	2.9925	-0.9225
C	-1.0548	-0.1686	-0.0342	C	0.9282	-1.7485	0.1258	H	3.2686	2.4567	0.6751
C	-1.5556	1.1350	0.2621	C	2.2934	-1.9684	-0.1364	H	5.6849	2.0455	0.5526
C	0.7119	2.0348	-0.1129	C	2.7915	-3.2856	-0.2244	H	6.5518	-0.1756	-0.1709
C	-0.6394	2.2600	0.2079	C	1.9872	-4.3655	0.0581	H	4.9555	-2.0524	-0.5374
C	-1.1263	3.5749	0.3161	C	0.6681	-4.1464	0.4754	H	3.8467	-3.4341	-0.4998
C	-0.3283	4.6537	-0.0062	C	0.1567	-2.8679	0.5092	H	2.3768	-5.3858	-0.0146
C	0.9635	4.4279	-0.4861	H	-6.3618	-2.5332	-0.6709	H	0.0455	-4.9961	0.7744
C	1.4680	3.1426	-0.5394	H	-7.1932	-0.3680	0.1955	H	-0.8794	-2.7249	0.8450

Table 3.447: Table of thermodynamic data as a function of temperature for Tribenzo[*b,g,p*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.098	561.824	561.824	∞
100	126.594	374.564	868.205	-49.364	591.402	647.456	-338.189
200	246.779	497.219	652.136	-30.983	575.756	709.746	-185.363
250	316.793	559.745	627.377	-16.908	568.388	744.096	-155.467
298.15	385.391	621.419	621.419	0.000	561.824	778.549	-136.396
300	388.000	623.811	621.426	0.715	561.582	779.893	-135.789
350	456.676	688.829	626.404	21.849	555.545	816.769	-121.894
400	520.452	754.036	638.284	46.301	550.323	854.443	-111.576
450	578.252	818.734	654.748	73.794	545.828	892.733	-103.624
500	629.915	882.386	674.339	104.023	541.959	931.513	-97.312
600	716.525	1005.203	719.340	171.518	535.752	1010.041	-87.930
700	785.009	1120.999	768.536	246.725	531.327	1089.469	-81.295
800	839.960	1229.539	819.452	328.070	528.466	1169.404	-76.353
900	884.784	1331.146	870.724	414.380	526.960	1249.609	-72.524
1000	921.857	1426.346	921.577	504.769	526.623	1329.931	-69.467
1100	952.856	1515.705	971.569	598.550	527.232	1410.250	-66.966
1200	978.999	1599.767	1020.451	695.179	528.629	1490.457	-64.877
1300	1001.204	1679.029	1068.092	794.218	530.610	1570.536	-63.104
1400	1020.182	1753.939	1114.430	895.312	533.028	1650.449	-61.578
1500	1036.494	1824.894	1159.450	998.166	535.790	1730.179	-60.249
1600	1050.587	1892.249	1203.163	1102.537	538.752	1809.707	-59.080
1700	1062.824	1956.316	1245.597	1208.222	541.830	1889.019	-58.041
1800	1073.501	2017.374	1286.791	1315.050	544.943	1968.220	-57.115
1900	1082.858	2075.672	1326.789	1422.878	548.053	2047.189	-56.280
2000	1091.095	2131.429	1365.637	1531.584	551.099	2126.025	-55.525
2100	1098.376	2184.843	1403.384	1641.065	553.996	2204.696	-54.838
2200	1104.836	2236.092	1440.077	1751.232	556.742	2283.236	-54.210
2300	1110.591	2285.333	1475.764	1862.009	559.330	2361.653	-53.634
2400	1115.737	2332.710	1510.490	1973.330	561.682	2439.909	-53.102
2500	1120.352	2378.352	1544.297	2085.139	563.810	2518.197	-52.614
2600	1124.506	2422.376	1577.227	2197.385	565.675	2596.276	-52.159
2700	1128.257	2464.886	1609.321	2310.026	567.280	2674.367	-51.738
2800	1131.653	2505.981	1640.615	2423.025	568.597	2752.430	-51.346
2900	1134.737	2545.747	1671.144	2536.347	569.593	2830.391	-50.980
3000	1137.545	2584.264	1700.943	2649.963	570.317	2908.352	-50.638
3100	1140.109	2621.606	1730.043	2763.848	570.681	2986.210	-50.316
3200	1142.455	2657.841	1758.473	2877.977	570.733	3064.142	-50.016
3300	1144.606	2693.030	1786.262	2992.332	570.452	3142.120	-49.735
3400	1146.585	2727.229	1813.437	3106.893	569.807	3220.018	-49.469
3500	1148.407	2760.493	1840.023	3221.644	568.803	3297.919	-49.218
3600	1150.089	2792.868	1866.043	3336.570	567.463	3375.949	-48.983
3700	1151.645	2824.401	1891.520	3451.657	565.755	3454.042	-48.761
3800	1153.086	2855.133	1916.476	3566.895	563.648	3532.118	-48.551
3900	1154.425	2885.102	1940.930	3682.271	561.187	3610.199	-48.352
4000	1155.669	2914.345	1964.901	3797.777	558.354	3688.501	-48.166
4100	1156.828	2942.896	1988.408	3913.402	555.111	3766.795	-47.989
4200	1157.909	2970.786	2011.467	4029.140	551.487	3845.165	-47.821
4300	1158.919	2998.044	2034.095	4144.982	547.467	3923.525	-47.660
4400	1159.864	3024.698	2056.307	4260.921	543.062	4002.086	-47.510
4500	1160.749	3050.774	2078.118	4376.952	538.286	4080.814	-47.368
4600	1161.580	3076.295	2099.541	4493.069	533.083	4159.659	-47.233
4700	1162.360	3101.285	2120.589	4609.267	527.468	4238.497	-47.105
4800	1163.093	3125.764	2141.276	4725.540	521.494	4317.575	-46.984
4900	1163.784	3149.753	2161.614	4841.884	515.079	4396.632	-46.868
5000	1164.435	3173.271	2181.612	4958.295	508.325	4476.033	-46.760

3.448. Dibenzo[*f,s*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-72-3
Point Group: C₁

Length: 14.67 Å
Width: 11.65 Å
Breadth: 6.817 Å
L/B Ratio: 1.259

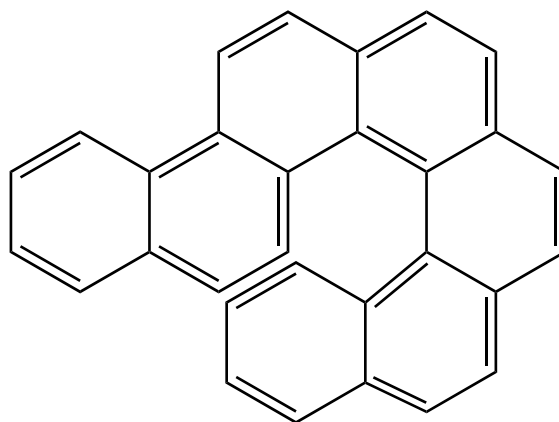
Cartesian coordinates:

C	5.4331	-0.3415	0.8349	C	-0.9333	-0.7575	-0.0518	H	5.0452	3.0325	1.0565
C	5.7699	1.0112	1.0344	C	-0.5885	0.5812	-0.2053	H	3.9269	-1.7580	0.3106
C	4.8084	1.9761	0.8849	C	-2.2498	-1.0897	0.4641	H	2.7532	3.6653	0.6722
C	4.1633	-0.6949	0.4556	C	-3.2526	-0.1040	0.4835	H	0.4130	3.0634	0.2234
C	3.1501	0.2782	0.2502	C	-4.5087	-0.3898	1.0523	H	-1.3900	-3.3509	-0.7358
C	3.4862	1.6214	0.5182	C	-4.7624	-1.6198	1.6189	H	0.2292	-4.9006	-1.7724
C	2.4770	2.6247	0.4658	C	-3.7607	-2.5978	1.6271	H	2.5847	-4.1803	-2.1405
C	1.1884	2.2851	0.2053	C	-2.5324	-2.3376	1.0574	H	3.3285	-1.9506	-1.3914
C	1.8014	-0.0474	-0.1470	C	-2.9796	1.1964	-0.0928	H	-5.2836	0.3918	1.0334
C	0.8121	0.9401	-0.0946	C	-1.6583	1.5415	-0.4300	H	-5.7387	-1.8342	2.0653
C	1.3965	-1.3675	-0.5911	C	-1.4437	2.7703	-1.0881	H	-3.9561	-3.5708	2.0898
C	0.0453	-1.7466	-0.4518	C	-2.4840	3.6372	-1.3483	H	-1.7576	-3.1168	1.0620
C	-0.3446	-3.0388	-0.8674	C	-3.7873	3.3113	-0.9551	H	-0.4260	3.0418	-1.4006
C	0.5522	-3.9062	-1.4478	C	-4.0288	2.1031	-0.3386	H	-2.2938	4.5830	-1.8662
C	1.8791	-3.5047	-1.6462	H	6.1963	-1.1115	0.9895	H	-4.6076	4.0099	-1.1484
C	2.2873	-2.2595	-1.2247	H	6.7928	1.2779	1.3188	H	-5.0480	1.8222	-0.0317

Table 3.448: Table of thermodynamic data as a function of temperature for Dibenzo[*f,s*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.888	554.897	554.897	∞
100	126.167	367.708	860.885	-49.318	584.522	641.261	-334.954
200	246.621	490.237	645.005	-30.954	568.860	704.246	-183.926
250	316.482	552.710	620.271	-16.890	561.479	738.947	-154.391
298.15	384.968	614.319	614.319	0.000	554.897	773.740	-135.553
300	387.573	616.708	614.326	0.715	554.655	775.096	-134.953
350	456.199	681.657	619.299	21.825	548.595	812.330	-121.231
400	519.972	746.799	631.167	46.253	543.349	850.363	-111.044
450	577.794	811.442	647.613	73.723	538.830	889.017	-103.192
500	629.491	875.047	667.187	103.930	534.939	928.162	-96.962
600	716.173	997.793	712.150	171.386	528.694	1007.428	-87.703
700	784.718	1113.540	761.311	246.560	524.237	1087.600	-81.156
800	839.717	1222.044	812.195	327.879	521.349	1168.283	-76.279
900	884.577	1323.625	863.439	414.167	519.820	1249.238	-72.502
1000	921.679	1418.804	914.268	504.537	519.464	1330.314	-69.487
1100	952.701	1508.148	964.238	598.301	520.057	1411.388	-67.020
1200	978.862	1592.197	1013.101	694.915	521.440	1492.352	-64.959
1300	1001.083	1671.449	1060.724	793.942	523.407	1573.188	-63.210
1400	1020.073	1746.350	1107.047	895.024	525.814	1653.860	-61.705
1500	1036.396	1817.298	1152.053	997.868	528.565	1734.349	-60.394
1600	1050.498	1884.647	1195.753	1102.229	531.518	1814.637	-59.241
1700	1062.744	1948.709	1238.176	1207.906	534.588	1894.709	-58.216
1800	1073.428	2009.763	1279.359	1314.726	537.693	1974.671	-57.302
1900	1082.791	2068.056	1319.347	1422.547	540.796	2054.402	-56.478
2000	1091.033	2123.810	1358.187	1531.247	543.835	2133.999	-55.733
2100	1098.319	2177.222	1395.926	1640.722	546.726	2213.432	-55.055
2200	1104.784	2228.468	1432.612	1750.883	549.467	2292.734	-54.435
2300	1110.543	2277.707	1468.291	1861.655	552.050	2371.914	-53.867
2400	1115.691	2325.082	1503.010	1972.972	554.397	2450.933	-53.342
2500	1120.310	2370.722	1536.812	2084.776	556.521	2529.984	-52.860
2600	1124.467	2414.744	1569.737	2197.018	558.382	2608.826	-52.411
2700	1128.220	2457.253	1601.825	2309.656	559.983	2687.680	-51.995
2800	1131.619	2498.346	1633.114	2422.650	561.297	2766.506	-51.609
2900	1134.705	2538.111	1663.639	2535.969	562.289	2845.231	-51.247
3000	1137.515	2576.627	1693.433	2649.582	563.010	2923.955	-50.910
3100	1140.080	2613.969	1722.529	2763.464	563.371	3002.577	-50.592
3200	1142.428	2650.202	1750.955	2877.591	563.420	3081.273	-50.296
3300	1144.581	2685.390	1778.741	2991.943	563.136	3160.015	-50.018
3400	1146.560	2719.589	1805.912	3106.501	562.489	3238.676	-49.755
3500	1148.384	2752.852	1832.494	3221.250	561.482	3317.342	-49.508
3600	1150.067	2785.226	1858.512	3336.174	560.141	3396.136	-49.276
3700	1151.624	2816.759	1883.986	3451.259	558.430	3474.994	-49.057
3800	1153.067	2847.490	1908.939	3566.495	556.321	3553.834	-48.850
3900	1154.406	2877.459	1933.390	3681.869	553.858	3632.679	-48.653
4000	1155.651	2906.702	1957.359	3797.373	551.024	3711.745	-48.469
4100	1156.811	2935.252	1980.863	3912.996	547.779	3790.804	-48.294
4200	1157.893	2963.142	2003.920	4028.732	544.154	3869.938	-48.129
4300	1158.904	2990.399	2026.545	4144.573	540.132	3949.063	-47.971
4400	1159.849	3017.053	2048.755	4260.511	535.725	4028.388	-47.822
4500	1160.735	3043.128	2070.564	4376.540	530.948	4107.880	-47.682
4600	1161.566	3068.649	2091.985	4492.656	525.743	4187.490	-47.549
4700	1162.346	3093.638	2113.032	4608.852	520.127	4267.092	-47.422
4800	1163.080	3118.118	2133.717	4725.124	514.152	4346.935	-47.303
4900	1163.772	3142.107	2154.052	4841.467	507.735	4426.757	-47.189
5000	1164.423	3165.625	2174.049	4957.877	500.980	4506.922	-47.083

3.449. Phenanthro[3,4-*c*]chrysene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 31124-69-3
Point Group: C_1

Length: 14.00 Å
Width: 11.12 Å
Breadth: 7.508 Å
L/B Ratio: 1.260

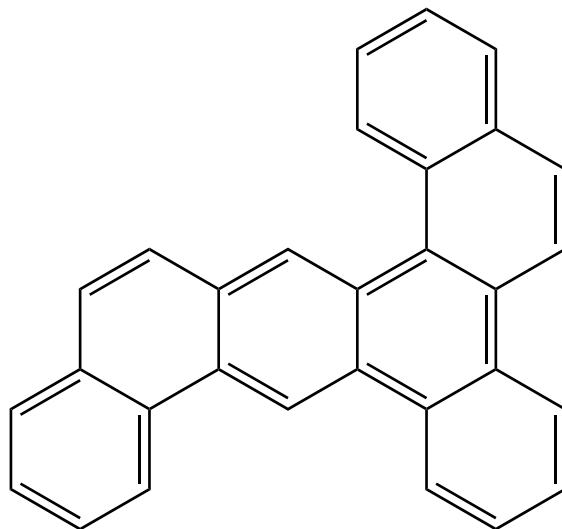
Cartesian coordinates:

C	0.7241	3.8986	-1.2302	C	0.5513	-2.7631	-0.5600	H	-1.1246	1.7854	-3.1321
C	-0.2243	3.4819	-2.1322	C	0.5868	-1.4405	-0.0890	H	0.2119	0.1101	-1.9072
C	-0.3934	2.1093	-2.3841	C	-1.8623	-2.7252	-0.6585	H	4.3414	2.8426	1.3874
C	0.3508	1.1787	-1.6989	C	-0.6895	-3.3728	-0.8990	H	2.7058	4.4802	0.4710
C	1.5209	2.9547	-0.5426	C	-1.8680	-1.4782	0.0282	H	5.0529	-1.8031	0.8747
C	1.3016	1.5744	-0.7282	C	-0.6539	-0.8566	0.3513	H	5.2225	0.6125	1.4709
C	3.4734	2.5110	0.8059	C	-0.6817	0.2937	1.2062	H	1.6946	-4.5621	-1.0165
C	2.5921	3.4047	0.2945	C	-1.8512	0.8358	1.6307	H	3.8287	-3.6253	-0.1283
C	3.2867	1.1055	0.6041	C	-3.1179	-0.8807	0.4312	H	-2.8282	-3.1689	-0.9440
C	2.1209	0.6221	-0.0073	C	-3.1048	0.2790	1.2255	H	-0.6803	-4.3694	-1.3552
C	4.2192	-1.1154	0.6936	C	-4.3254	0.8725	1.6233	H	0.2731	0.7289	1.5289
C	4.3237	0.2095	0.9906	C	-5.5223	0.3207	1.2361	H	-1.8565	1.7095	2.2925
C	2.9972	-1.6361	0.1810	C	-5.5409	-0.8429	0.4441	H	-4.3004	1.7765	2.2422
C	1.8787	-0.7988	0.0258	C	-4.3644	-1.4331	0.0520	H	-6.4692	0.7788	1.5394
C	1.7513	-3.5341	-0.6411	H	0.8843	4.9666	-1.0435	H	-6.5022	-1.2726	0.1442
C	2.9206	-3.0145	-0.1851	H	-0.8414	4.2104	-2.6678	H	-4.3683	-2.3458	-0.5630

Table 3.449: Table of thermodynamic data as a function of temperature for Phenanthro[3,4-*c*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.993	547.617	547.617	∞
100	125.028	370.813	864.128	-49.331	577.228	633.657	-330.982
200	246.782	492.724	647.965	-31.048	561.485	696.374	-181.870
250	317.530	555.337	623.148	-16.953	554.137	730.947	-152.720
298.15	386.454	617.173	617.173	0.000	547.617	765.609	-134.129
300	389.070	619.571	617.180	0.717	547.378	766.960	-133.537
350	457.821	684.763	622.172	21.907	541.396	804.044	-119.995
400	521.545	750.120	634.083	46.415	536.231	841.917	-109.941
450	579.242	814.941	650.585	73.961	531.788	880.400	-102.192
500	630.797	878.692	670.219	104.237	527.966	919.367	-96.044
600	717.228	1001.653	715.303	171.810	521.838	998.256	-86.904
700	785.602	1117.549	764.576	247.081	517.477	1078.034	-80.442
800	840.490	1226.163	815.560	328.482	514.671	1158.311	-75.628
900	885.276	1327.830	866.893	414.843	513.217	1238.850	-71.899
1000	922.323	1423.080	917.800	505.280	512.927	1319.501	-68.922
1100	953.300	1512.483	967.841	599.106	513.582	1400.144	-66.486
1200	979.422	1596.582	1016.767	695.778	515.023	1480.672	-64.451
1300	1001.606	1675.877	1064.447	794.859	517.045	1561.068	-62.723
1400	1020.562	1750.816	1110.822	895.992	519.501	1641.295	-61.236
1500	1036.852	1821.797	1155.875	998.883	522.300	1721.336	-59.941
1600	1050.925	1889.174	1199.619	1103.289	525.297	1801.172	-58.801
1700	1063.142	1953.261	1242.081	1209.006	528.409	1880.790	-57.788
1800	1073.799	2014.337	1283.301	1315.865	531.552	1960.296	-56.885
1900	1083.138	2072.650	1323.323	1423.722	534.691	2039.568	-56.070
2000	1091.358	2128.421	1362.194	1532.456	537.764	2118.705	-55.334
2100	1098.622	2181.848	1399.962	1641.962	540.686	2197.676	-54.663
2200	1105.068	2233.108	1436.675	1752.153	543.456	2276.515	-54.050
2300	1110.809	2282.359	1472.380	1862.952	546.066	2355.230	-53.488
2400	1115.941	2329.745	1507.123	1974.294	548.440	2433.783	-52.969
2500	1120.545	2375.395	1540.946	2086.123	550.588	2512.367	-52.492
2600	1124.688	2419.426	1573.892	2198.388	552.471	2590.741	-52.048
2700	1128.428	2461.943	1606.000	2311.047	554.094	2669.128	-51.636
2800	1131.815	2503.044	1637.307	2424.062	555.428	2747.484	-51.254
2900	1134.890	2542.815	1667.850	2537.399	556.440	2825.739	-50.896
3000	1137.690	2581.338	1697.661	2651.030	557.178	2903.992	-50.562
3100	1140.246	2618.684	1726.772	2764.929	557.556	2982.142	-50.248
3200	1142.584	2654.923	1755.213	2879.072	557.622	3060.366	-49.954
3300	1144.730	2690.116	1783.013	2993.439	557.353	3138.637	-49.679
3400	1146.702	2724.319	1810.198	3108.012	556.720	3216.825	-49.419
3500	1148.518	2757.586	1836.793	3222.775	555.727	3295.017	-49.174
3600	1150.195	2789.964	1862.822	3337.711	554.399	3373.338	-48.945
3700	1151.746	2821.500	1888.308	3452.809	552.701	3451.722	-48.729
3800	1153.183	2852.234	1913.272	3568.057	550.603	3530.087	-48.523
3900	1154.517	2882.206	1937.734	3683.443	548.152	3608.458	-48.329
4000	1155.757	2911.452	1961.713	3798.957	545.328	3687.049	-48.147
4100	1156.912	2940.005	1985.227	3914.591	542.093	3765.633	-47.974
4200	1157.990	2967.897	2008.293	4030.337	538.478	3844.291	-47.810
4300	1158.996	2995.157	2030.927	4146.187	534.466	3922.941	-47.653
4400	1159.938	3021.812	2053.146	4262.134	530.068	4001.790	-47.506
4500	1160.820	3047.889	2074.962	4378.172	525.300	4080.806	-47.368
4600	1161.648	3073.412	2096.391	4494.296	520.103	4159.940	-47.237
4700	1162.425	3098.403	2117.446	4610.500	514.496	4239.066	-47.111
4800	1163.156	3122.884	2138.138	4726.780	508.528	4318.432	-46.993
4900	1163.844	3146.875	2158.481	4843.130	502.118	4397.777	-46.880
5000	1164.493	3170.394	2178.485	4959.547	495.371	4477.466	-46.775

3.450. Phenanthro[2,3-g]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-40-5
Point Group: C₁

Length: 16.25 Å
Width: 12.54 Å
Breadth: 5.057 Å
L/B Ratio: 1.295

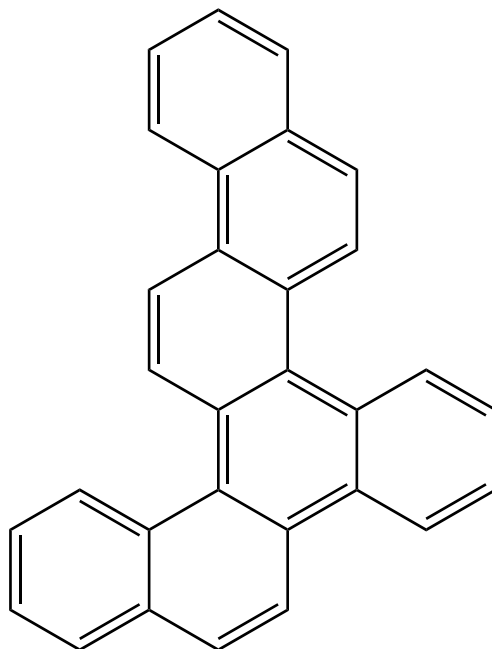
Cartesian coordinates:

C	5.8477	-1.4344	-0.1494	C	0.1529	3.4869	0.3482	H	6.4474	1.8399	0.5351
C	6.5538	-0.2801	0.1122	C	-0.5197	4.6905	0.3003	H	3.9503	1.9086	0.4496
C	5.8758	0.9290	0.3298	C	-1.8905	4.7106	0.0221	H	1.7730	-3.5084	-0.7277
C	4.4996	0.9688	0.2846	C	-2.5707	3.5276	-0.1834	H	4.2537	-3.5362	-0.6507
C	4.4392	-1.4105	-0.1989	C	-1.9864	-0.1893	-0.0517	H	2.1360	1.9427	0.3053
C	3.7585	-0.2007	0.0216	C	-2.6309	1.0327	-0.2381	H	-0.3087	-2.3157	-0.5064
C	2.3419	-2.5955	-0.5163	C	-4.0273	1.0705	-0.5211	H	1.2348	3.4607	0.5494
C	3.6936	-2.6105	-0.4750	C	-4.7725	-0.0663	-0.5405	H	0.0153	5.6297	0.4736
C	1.6094	-1.3779	-0.2822	C	-2.8009	-1.3677	0.1272	H	-2.4212	5.6669	-0.0281
C	2.3112	-0.1820	-0.0273	C	-4.1809	-1.3053	-0.1656	H	-3.6500	3.5456	-0.3963
C	1.5825	0.9976	0.1434	C	-4.9972	-2.4586	-0.0422	H	-4.4929	2.0437	-0.7382
C	0.2102	-1.3684	-0.2980	C	-4.4736	-3.6339	0.4271	H	-5.8360	-0.0410	-0.8040
C	-0.5256	-0.2074	-0.0596	C	-3.1176	-3.6872	0.8065	H	-6.0559	-2.3889	-0.3175
C	0.1903	1.0092	0.0957	C	-2.3099	-2.5893	0.6605	H	-5.0982	-4.5273	0.5258
C	-1.9057	2.2880	-0.1178	H	6.3740	-2.3802	-0.3214	H	-2.7156	-4.6156	1.2258
C	-0.5247	2.2732	0.1289	H	7.6479	-0.2996	0.1512	H	-1.2596	-2.6551	0.9758

Table 3.450: Table of thermodynamic data as a function of temperature for Phenanthro[2,3-g]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-57.348	509.560	509.560	∞
100	127.598	378.695	873.377	-49.468	539.034	594.675	-310.620
200	247.299	501.803	656.926	-31.025	523.452	656.525	-171.463
250	317.225	564.437	632.137	-16.925	516.107	690.643	-144.299
298.15	385.656	626.173	626.173	0.000	509.560	724.868	-126.991
300	388.258	628.567	626.181	0.716	509.319	726.203	-126.441
350	456.734	693.610	631.161	21.857	503.289	762.841	-113.845
400	520.331	758.812	643.044	46.307	498.066	800.275	-104.503
450	577.994	823.488	659.508	73.791	493.561	838.327	-97.308
500	629.564	887.107	679.098	104.005	489.677	876.870	-91.604
600	716.091	1009.851	724.086	171.459	483.430	954.929	-83.132
700	784.580	1125.581	773.263	246.622	478.962	1033.896	-77.149
800	839.573	1234.066	824.157	327.927	476.059	1113.376	-72.694
900	884.451	1335.630	875.407	414.201	474.517	1193.130	-69.246
1000	921.579	1430.798	926.239	504.559	474.149	1273.006	-66.494
1100	952.625	1520.133	976.210	598.314	474.734	1352.881	-64.242
1200	978.808	1604.176	1025.074	694.922	476.110	1432.646	-62.360
1300	1001.047	1683.424	1072.698	793.945	478.073	1512.285	-60.763
1400	1020.052	1758.324	1119.021	895.024	480.476	1591.759	-59.388
1500	1036.385	1829.271	1164.027	997.866	483.227	1671.051	-58.190
1600	1050.496	1896.619	1207.727	1102.227	486.179	1750.142	-57.135
1700	1062.748	1960.681	1250.150	1207.904	489.249	1829.017	-56.198
1800	1073.437	2021.736	1291.333	1314.725	492.354	1907.781	-55.361
1900	1082.804	2080.030	1331.321	1422.547	495.458	1986.315	-54.606
2000	1091.048	2135.784	1370.160	1531.248	498.500	2064.715	-53.924
2100	1098.335	2189.197	1407.899	1640.725	501.392	2142.950	-53.302
2200	1104.801	2240.443	1444.585	1750.888	504.134	2221.055	-52.733
2300	1110.561	2289.683	1480.265	1861.662	506.719	2299.037	-52.212
2400	1115.710	2337.059	1514.984	1972.980	509.068	2376.858	-51.730
2500	1120.329	2382.700	1548.786	2084.786	511.194	2454.712	-51.287
2600	1124.485	2426.722	1581.711	2197.030	513.056	2532.356	-50.875
2700	1128.238	2469.232	1613.799	2309.669	514.660	2610.012	-50.493
2800	1131.637	2510.326	1645.088	2422.666	515.975	2687.641	-50.138
2900	1134.722	2550.091	1675.613	2535.986	516.970	2765.167	-49.805
3000	1137.532	2588.608	1705.408	2649.601	517.691	2842.693	-49.495
3100	1140.097	2625.950	1734.504	2763.485	518.055	2920.117	-49.203
3200	1142.444	2662.185	1762.930	2877.613	518.106	2997.614	-48.930
3300	1144.597	2697.373	1790.716	2991.967	517.823	3075.159	-48.675
3400	1146.575	2731.572	1817.888	3106.527	517.177	3152.622	-48.433
3500	1148.399	2764.835	1844.471	3221.277	516.172	3230.088	-48.205
3600	1150.081	2797.211	1870.488	3336.202	514.832	3307.685	-47.992
3700	1151.638	2828.743	1895.962	3451.289	513.123	3385.344	-47.792
3800	1153.080	2859.475	1920.915	3566.526	511.015	3462.985	-47.601
3900	1154.419	2889.444	1945.367	3681.901	508.554	3540.632	-47.420
4000	1155.664	2918.687	1969.336	3797.406	505.720	3618.499	-47.252
4100	1156.823	2947.238	1992.840	3913.031	502.476	3696.360	-47.091
4200	1157.904	2975.128	2015.897	4028.768	498.852	3774.295	-46.939
4300	1158.915	3002.386	2038.523	4144.610	494.832	3852.221	-46.794
4400	1159.860	3029.040	2060.733	4260.549	490.426	3930.348	-46.658
4500	1160.745	3055.115	2082.542	4376.580	485.650	4008.641	-46.530
4600	1161.576	3080.636	2103.963	4492.696	480.446	4087.053	-46.409
4700	1162.356	3105.626	2125.010	4608.893	474.831	4165.456	-46.293
4800	1163.090	3130.105	2145.695	4725.166	468.857	4244.100	-46.184
4900	1163.781	3154.094	2166.031	4841.510	462.441	4322.723	-46.080
5000	1164.432	3177.612	2186.028	4957.921	455.687	4401.690	-45.983

3.451. Dibenzo[*a,f*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-36-9
Point Group: C₁

Length: 16.15 Å
Width: 12.21 Å
Breadth: 5.564 Å
L/B Ratio: 1.323

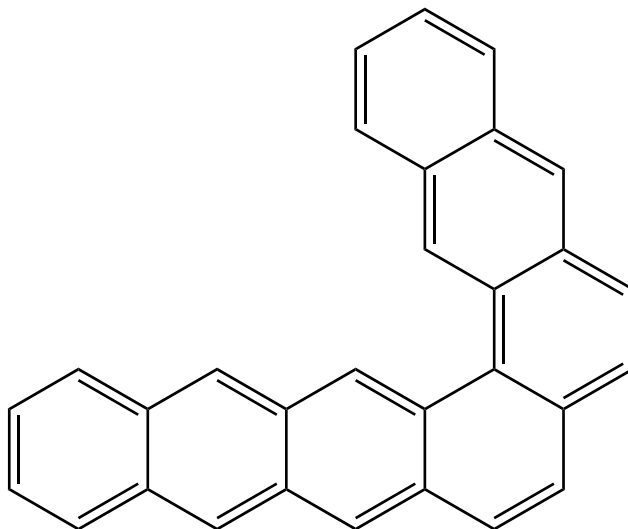
Cartesian coordinates:

C	-5.5933	2.4967	-0.0465	C	-0.3602	-3.1218	0.8252	H	-6.5975	-0.7498	-0.3299
C	-6.4536	1.3901	-0.1617	C	0.2204	-4.3725	0.8488	H	-3.5511	3.1764	0.0810
C	-5.9358	0.1187	-0.2360	C	1.4978	-4.5640	0.3092	H	-4.6573	-2.2426	-0.4377
C	-4.2313	2.3154	-0.0041	C	2.2026	-3.4803	-0.1659	H	-2.2437	-2.6101	-0.2856
C	-3.6742	1.0177	-0.0708	C	1.9987	0.2413	-0.0573	H	0.6420	2.5874	-0.1240
C	-4.5382	-0.0828	-0.1920	C	2.4713	-1.0270	-0.3901	H	-1.7895	2.9177	-0.0557
C	-3.9776	-1.3961	-0.2851	C	3.7928	-1.1977	-0.8981	H	-1.3637	-2.9902	1.2523
C	-2.6391	-1.5891	-0.1951	C	4.6520	-0.1479	-0.9691	H	-0.3171	-5.2200	1.2868
C	-2.2465	0.7982	-0.0178	C	2.9720	1.2989	0.0933	H	1.9383	-5.5658	0.2882
C	-1.7171	-0.5032	-0.0040	C	4.2768	1.1102	-0.4120	H	3.2244	-3.6057	-0.5556
C	-0.0137	1.7101	-0.0378	C	5.2397	2.1457	-0.3182	H	4.0934	-2.2017	-1.2341
C	-1.3642	1.9026	-0.0256	C	4.9410	3.3165	0.3291	H	5.6504	-0.2603	-1.4067
C	0.5566	0.4145	0.0523	C	3.6731	3.4808	0.9188	H	6.2313	1.9883	-0.7581
C	-0.3001	-0.6974	0.1226	C	2.7194	2.5013	0.8029	H	5.6821	4.1184	0.4073
C	1.6427	-2.1867	-0.1393	H	-6.0179	3.5044	0.0087	H	3.4563	4.3980	1.4763
C	0.3067	-2.0131	0.2655	H	-7.5361	1.5507	-0.1930	H	1.7412	2.6457	1.2817

Table 3.451: Table of thermodynamic data as a function of temperature for Dibenzo[*a,f*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.912	537.857	537.857	∞
100	125.680	371.943	864.617	-49.267	567.532	623.848	-325.858
200	246.381	494.091	648.874	-30.957	551.817	686.432	-179.274
250	316.545	556.548	624.135	-16.897	544.433	720.941	-150.629
298.15	385.148	618.179	618.179	0.000	537.857	755.549	-132.366
300	387.756	620.570	618.187	0.715	537.615	756.898	-131.785
350	456.375	685.547	623.162	21.835	531.564	793.938	-118.486
400	520.088	750.709	635.035	46.270	526.326	831.776	-108.617
450	577.839	815.362	651.487	73.744	521.811	870.234	-101.012
500	629.473	878.968	671.065	103.952	517.921	909.183	-94.980
600	716.073	1001.703	716.035	171.401	511.669	988.057	-86.016
700	784.586	1117.432	765.197	246.564	507.200	1067.839	-79.681
800	839.579	1225.917	816.081	327.869	504.298	1148.134	-74.964
900	884.448	1327.482	867.323	414.143	502.757	1228.703	-71.311
1000	921.564	1422.649	918.148	504.501	502.388	1309.393	-68.394
1100	952.601	1511.982	968.115	598.254	502.971	1390.083	-66.008
1200	978.776	1596.023	1016.974	694.859	504.344	1470.664	-64.015
1300	1001.009	1675.269	1064.593	793.878	506.304	1551.118	-62.323
1400	1020.010	1750.165	1110.912	894.953	508.703	1631.408	-60.867
1500	1036.341	1821.109	1155.915	997.791	511.449	1711.516	-59.599
1600	1050.451	1888.454	1199.612	1102.148	514.396	1791.423	-58.483
1700	1062.703	1952.514	1242.032	1207.820	517.462	1871.115	-57.491
1800	1073.392	2013.565	1283.212	1314.636	520.563	1950.696	-56.607
1900	1082.760	2071.857	1323.197	1422.454	523.662	2030.047	-55.809
2000	1091.005	2127.610	1362.034	1531.151	526.699	2109.264	-55.087
2100	1098.294	2181.020	1399.771	1640.623	529.587	2188.317	-54.430
2200	1104.762	2232.265	1436.455	1750.782	532.326	2267.240	-53.830
2300	1110.523	2281.503	1472.132	1861.552	534.906	2346.039	-53.279
2400	1115.673	2328.877	1506.849	1972.866	537.252	2424.679	-52.771
2500	1120.294	2374.516	1540.649	2084.669	539.374	2503.351	-52.304
2600	1124.452	2418.538	1573.572	2196.910	541.233	2581.813	-51.868
2700	1128.207	2461.046	1605.659	2309.546	542.833	2660.288	-51.465
2800	1131.606	2502.139	1636.946	2422.539	544.146	2738.735	-51.091
2900	1134.694	2541.903	1667.470	2535.857	545.137	2817.080	-50.740
3000	1137.505	2580.419	1697.263	2649.469	545.856	2895.425	-50.413
3100	1140.071	2617.760	1726.357	2763.349	546.217	2973.668	-50.105
3200	1142.419	2653.994	1754.783	2877.476	546.265	3051.984	-49.818
3300	1144.573	2689.181	1782.567	2991.827	545.980	3130.348	-49.548
3400	1146.553	2723.380	1809.738	3106.384	545.332	3208.630	-49.294
3500	1148.377	2756.642	1836.319	3221.132	544.324	3286.916	-49.054
3600	1150.061	2789.017	1862.335	3336.055	542.982	3365.332	-48.829
3700	1151.618	2820.549	1887.809	3451.140	541.271	3443.810	-48.617
3800	1153.061	2851.280	1912.760	3566.375	539.161	3522.271	-48.416
3900	1154.400	2881.249	1937.211	3681.749	536.698	3600.737	-48.225
4000	1155.646	2910.492	1961.179	3797.252	533.863	3679.424	-48.047
4100	1156.806	2939.042	1984.682	3912.875	530.617	3758.104	-47.878
4200	1157.888	2966.931	2007.738	4028.610	526.992	3836.859	-47.717
4300	1158.899	2994.189	2030.363	4144.450	522.970	3915.605	-47.564
4400	1159.845	3020.843	2052.573	4260.388	518.562	3994.551	-47.420
4500	1160.731	3046.918	2074.380	4376.417	513.785	4073.664	-47.285
4600	1161.562	3072.438	2095.801	4492.532	508.580	4152.896	-47.157
4700	1162.343	3097.428	2116.847	4608.728	502.963	4232.119	-47.034
4800	1163.077	3121.907	2137.532	4724.999	496.988	4311.583	-46.919
4900	1163.768	3145.896	2157.867	4841.342	490.570	4391.026	-46.808
5000	1164.420	3169.414	2177.863	4957.752	483.815	4470.812	-46.705

3.452. Anthra[1,2-*a*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-78-9
Point Group: C₁

Length: 16.57 Å
Width: 12.20 Å
Breadth: 5.055 Å
L/B Ratio: 1.358

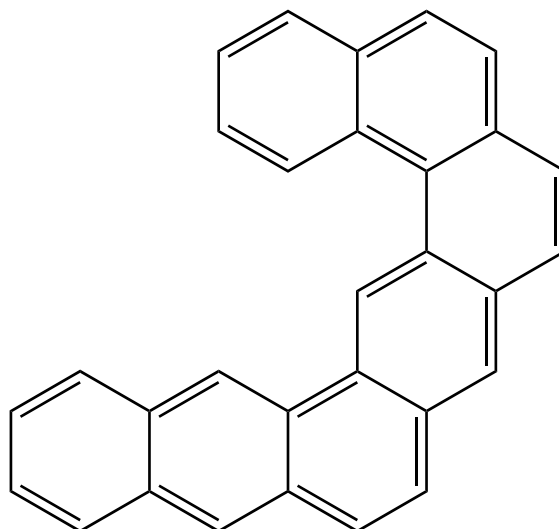
Cartesian coordinates:

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C	-6.8343	1.5968	-0.0391	C	1.8930	-2.9314	-0.0910	H	-4.0619	3.4120	-0.9057
C	-6.2678	0.3937	0.2307	C	3.2631	-3.2078	-0.4109	H	-4.8663	-1.8709	0.6830
C	-4.6865	2.5698	-0.5869	C	4.1415	-2.1993	-0.6111	H	-2.0519	2.0108	-0.7528
C	-4.0444	1.3136	-0.3103	C	2.3867	-0.5469	-0.0388	H	-2.8543	-3.2926	0.7180
C	-4.8480	0.2078	0.1033	C	3.7396	-0.8392	-0.3885	H	-0.0682	0.6367	-0.5784
C	-4.2530	-1.0170	0.3700	C	4.6945	0.1730	-0.4565	H	-0.9251	-4.7198	0.7013
C	-2.6708	1.1622	-0.4359	C	2.0898	0.7591	0.3504	H	1.4807	-5.0568	0.1844
C	-2.0582	-0.0751	-0.1570	C	3.0485	1.7796	0.3109	H	3.5733	-4.2543	-0.5143
C	-2.8606	-1.1775	0.2397	C	4.3648	1.4917	-0.1255	H	5.1777	-2.3982	-0.9080
C	-2.2324	-2.4249	0.4639	C	5.3272	2.5483	-0.1881	H	5.7228	-0.0669	-0.7552
C	-0.6545	-0.2365	-0.2562	C	4.9837	3.8132	0.1803	H	1.0819	1.0154	0.7086
C	-0.0303	-1.4343	0.0350	C	3.6658	4.1011	0.6346	H	6.3395	2.3142	-0.5362
C	-0.8647	-2.5648	0.3393	C	2.7254	3.1186	0.7003	H	5.7141	4.6276	0.1351
C	-0.2757	-3.8761	0.4410	H	-6.5240	3.6575	-0.6649	H	3.4241	5.1275	0.9295
C	1.0340	-4.0556	0.1742	H	-7.9151	1.7434	0.0563	H	1.7089	3.3321	1.0497

Table 3.452: Table of thermodynamic data as a function of temperature for Anthra[1,2-*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.065	544.093	544.093	∞
100	124.800	375.086	869.092	-49.401	573.634	629.636	-328.881
200	247.191	497.086	652.591	-31.101	557.908	691.924	-180.708
250	318.087	559.808	627.732	-16.981	550.584	726.277	-151.744
298.15	387.055	621.747	621.747	0.000	544.093	760.721	-133.272
300	389.670	624.149	621.754	0.718	543.854	762.063	-132.684
350	458.374	689.431	626.753	21.937	537.902	798.916	-119.229
400	522.006	754.856	638.679	46.471	532.763	836.554	-109.240
450	579.606	819.726	655.199	74.037	528.340	874.798	-101.542
500	631.078	883.510	674.852	104.329	524.534	913.525	-95.433
600	717.405	1006.511	719.971	171.924	518.428	991.931	-86.353
700	785.743	1122.431	769.273	247.211	514.083	1071.222	-79.934
800	840.632	1231.064	820.282	328.626	511.291	1151.009	-75.152
900	885.433	1332.749	871.636	415.002	509.851	1231.057	-71.447
1000	922.498	1428.017	922.561	505.455	509.578	1311.216	-68.489
1100	953.488	1517.436	972.619	599.300	510.252	1391.364	-66.069
1200	979.619	1601.553	1021.560	695.991	511.711	1471.396	-64.047
1300	1001.806	1680.864	1069.254	795.092	513.753	1551.294	-62.330
1400	1020.763	1755.817	1115.642	896.245	516.230	1631.021	-60.853
1500	1037.049	1826.812	1160.708	999.156	519.049	1710.562	-59.566
1600	1051.116	1894.202	1204.464	1103.581	522.065	1789.896	-58.433
1700	1063.327	1958.300	1246.937	1209.317	525.195	1869.011	-57.427
1800	1073.977	2019.386	1288.167	1316.194	528.356	1948.012	-56.529
1900	1083.308	2077.709	1328.199	1424.069	531.513	2026.779	-55.719
2000	1091.519	2133.488	1367.079	1532.819	534.602	2105.410	-54.987
2100	1098.775	2186.923	1404.856	1642.341	537.541	2183.873	-54.320
2200	1105.213	2238.190	1441.578	1752.546	540.325	2262.205	-53.710
2300	1110.947	2287.447	1477.291	1863.360	542.950	2340.411	-53.151
2400	1116.072	2334.839	1512.041	1974.715	545.336	2418.455	-52.635
2500	1120.668	2380.494	1545.871	2086.557	547.497	2496.530	-52.161
2600	1124.805	2424.529	1578.824	2198.834	549.393	2574.394	-51.719
2700	1128.539	2467.051	1610.939	2311.504	551.027	2652.269	-51.310
2800	1131.920	2508.156	1642.252	2424.530	552.372	2730.115	-50.930
2900	1134.990	2547.931	1672.800	2537.878	553.394	2807.858	-50.574
3000	1137.785	2586.456	1702.617	2651.519	554.142	2885.600	-50.242
3100	1140.336	2623.806	1731.733	2765.427	554.530	2963.238	-49.929
3200	1142.670	2660.048	1760.180	2879.579	554.604	3040.949	-49.637
3300	1144.811	2695.243	1787.984	2993.954	554.343	3118.707	-49.364
3400	1146.779	2729.449	1815.174	3108.535	553.718	3196.383	-49.105
3500	1148.592	2762.717	1841.773	3223.305	552.733	3274.062	-48.862
3600	1150.266	2795.098	1867.807	3338.249	551.412	3351.870	-48.633
3700	1151.814	2826.636	1893.297	3453.354	549.721	3429.739	-48.418
3800	1153.248	2857.372	1918.264	3568.608	547.630	3507.592	-48.214
3900	1154.579	2887.345	1942.730	3684.000	545.185	3585.448	-48.021
4000	1155.816	2916.593	1966.712	3799.521	542.367	3663.525	-47.840
4100	1156.969	2945.147	1990.230	3915.160	539.138	3741.595	-47.668
4200	1158.044	2973.040	2013.299	4030.912	535.529	3819.739	-47.504
4300	1159.048	3000.301	2035.937	4146.767	531.522	3897.874	-47.349
4400	1159.988	3026.958	2058.158	4262.719	527.129	3976.209	-47.203
4500	1160.868	3053.036	2079.978	4378.763	522.366	4054.711	-47.065
4600	1161.694	3078.560	2101.410	4494.891	517.174	4133.330	-46.934
4700	1162.470	3103.552	2122.467	4611.100	511.571	4211.941	-46.810
4800	1163.199	3128.034	2143.162	4727.384	505.607	4290.792	-46.692
4900	1163.886	3152.025	2163.507	4843.738	499.202	4369.622	-46.580
5000	1164.533	3175.546	2183.514	4960.159	492.458	4448.795	-46.475

3.453. Naphtho[1,2-*a*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-85-8
Point Group: C₁

Length: 15.60 Å
Width: 11.64 Å
Breadth: 5.258 Å
L/B Ratio: 1.340

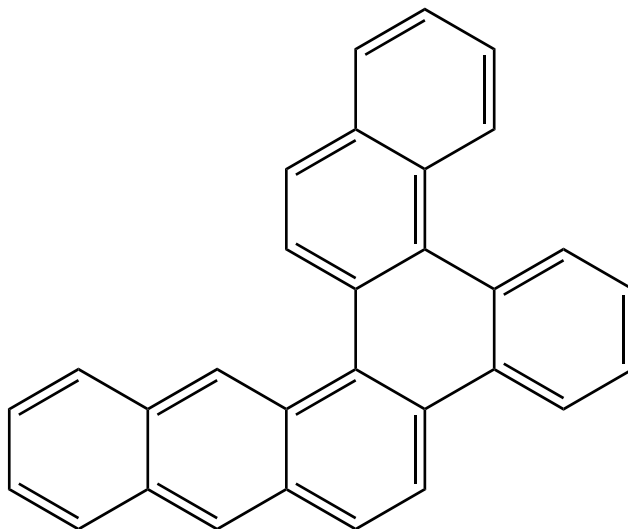
Cartesian coordinates:

C	-5.0609	-3.0472	0.4095	C	1.6984	1.0483	-0.0279	H	-6.8638	-0.1651	0.0387
C	-6.1807	-2.1834	0.2904	C	1.8265	2.4588	-0.0760	H	-2.9216	-3.2056	0.4586
C	-6.0049	-0.8393	0.1313	C	3.1152	3.0697	0.0621	H	-5.3519	1.7629	-0.1723
C	-3.7920	-2.5463	0.3663	C	4.2031	2.3042	0.3122	H	-1.4038	-1.2745	0.2421
C	-3.5760	-1.1463	0.2006	C	2.8967	0.2306	0.0363	H	-3.8802	3.6789	-0.3875
C	-4.6913	-0.2857	0.0826	C	4.1036	0.8747	0.3270	H	-1.5976	4.6448	-0.4536
C	-4.4834	1.0988	-0.0806	C	5.2811	0.1299	0.6427	H	0.8166	4.3636	-0.2672
C	-2.2756	-0.6060	0.1527	C	5.2665	-1.2264	0.6191	H	0.2411	-0.5617	0.1692
C	-2.0748	0.7545	-0.0056	C	2.9351	-1.2001	-0.1782	H	3.1904	4.1612	-0.0018
C	-3.2015	1.6195	-0.1247	C	4.1006	-1.9179	0.1694	H	5.1847	2.7607	0.4857
C	-2.9933	3.0417	-0.2922	C	4.1486	-3.3258	0.0236	H	6.1893	0.6772	0.9212
C	-1.7536	3.5670	-0.3284	C	3.0909	-4.0063	-0.5230	H	6.1498	-1.8084	0.9057
C	-0.7341	1.3254	-0.0573	C	1.9613	-3.2923	-0.9621	H	5.0507	-3.8612	0.3416
C	-0.5835	2.7270	-0.2023	C	1.8888	-1.9316	-0.7949	H	3.1229	-5.0945	-0.6372
C	0.6904	3.2757	-0.1955	H	-5.2331	-4.1210	0.5370	H	1.1411	-3.8318	-1.4474
C	0.3963	0.5233	0.0318	H	-7.1866	-2.6140	0.3286	H	1.0026	-1.4009	-1.1692

Table 3.453: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*a*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.053	511.077	511.077	∞
100	125.216	376.500	869.682	-49.318	540.700	596.561	-311.605
200	246.722	498.518	653.624	-31.021	524.971	658.701	-172.032
250	317.243	561.093	628.830	-16.934	517.614	692.986	-144.789
298.15	385.987	622.862	622.862	0.000	511.077	727.372	-127.430
300	388.597	625.258	622.869	0.716	510.836	728.712	-126.877
350	457.204	690.365	627.855	21.879	504.827	765.514	-114.244
400	520.827	755.633	639.750	46.353	499.629	803.109	-104.873
450	578.467	820.366	656.230	73.861	495.148	841.319	-97.656
500	630.001	884.033	675.837	104.098	491.286	880.017	-91.933
600	716.468	1006.851	720.863	171.592	485.080	958.380	-83.433
700	784.930	1122.635	770.076	246.792	480.647	1037.643	-77.428
800	839.921	1231.167	821.003	328.131	477.779	1117.416	-72.958
900	884.804	1332.773	872.284	414.440	476.273	1197.457	-69.497
1000	921.936	1427.978	923.144	504.834	475.941	1277.617	-66.734
1100	952.984	1517.347	973.142	598.625	476.561	1357.772	-64.474
1200	979.163	1601.421	1022.031	695.269	477.972	1437.815	-62.585
1300	1001.393	1680.698	1069.677	794.326	479.971	1517.727	-60.982
1400	1020.387	1755.622	1116.022	895.440	482.408	1597.473	-59.601
1500	1036.706	1826.592	1161.049	998.315	485.191	1677.034	-58.398
1600	1050.802	1893.960	1204.769	1102.707	488.174	1756.392	-57.339
1700	1063.039	1958.041	1247.209	1208.413	491.275	1835.532	-56.398
1800	1073.712	2019.111	1288.410	1315.263	494.408	1914.559	-55.558
1900	1083.063	2077.420	1328.414	1423.111	497.539	1993.354	-54.800
2000	1091.293	2133.187	1367.268	1531.838	500.605	2072.015	-54.114
2100	1098.566	2186.611	1405.022	1641.338	503.522	2150.509	-53.490
2200	1105.019	2237.868	1441.721	1751.524	506.286	2228.872	-52.919
2300	1110.766	2287.118	1477.414	1862.318	508.892	2307.111	-52.395
2400	1115.903	2334.502	1512.145	1973.657	511.261	2385.188	-51.911
2500	1120.511	2380.150	1545.958	2085.481	513.406	2463.297	-51.467
2600	1124.658	2424.180	1578.894	2197.744	515.286	2541.196	-51.052
2700	1128.401	2466.696	1610.993	2310.400	516.906	2619.107	-50.669
2800	1131.791	2507.796	1642.292	2423.412	518.238	2696.988	-50.312
2900	1134.868	2547.566	1672.826	2536.747	519.247	2774.767	-49.978
3000	1137.670	2586.088	1702.629	2650.376	519.983	2852.546	-49.666
3100	1140.228	2623.434	1731.733	2764.273	520.360	2930.221	-49.373
3200	1142.568	2659.673	1760.168	2878.415	520.423	3007.970	-49.099
3300	1144.715	2694.865	1787.962	2992.780	520.153	3085.765	-48.843
3400	1146.688	2729.068	1815.141	3107.352	519.519	3163.479	-48.600
3500	1148.506	2762.334	1841.730	3222.113	518.524	3241.196	-48.371
3600	1150.183	2794.712	1867.754	3337.048	517.195	3319.042	-48.157
3700	1151.735	2826.247	1893.235	3452.145	515.496	3396.951	-47.955
3800	1153.173	2856.981	1918.194	3567.392	513.397	3474.842	-47.764
3900	1154.508	2886.953	1942.652	3682.777	510.945	3552.738	-47.583
4000	1155.748	2916.199	1966.626	3798.290	508.121	3630.854	-47.413
4100	1156.904	2944.751	1990.136	3913.923	504.885	3708.964	-47.252
4200	1157.982	2972.643	2013.198	4029.668	501.269	3787.147	-47.099
4300	1158.989	2999.903	2035.829	4145.517	497.256	3865.322	-46.953
4400	1159.931	3026.558	2058.044	4261.464	492.858	3943.697	-46.817
4500	1160.814	3052.635	2079.857	4377.502	488.088	4022.238	-46.688
4600	1161.642	3078.158	2101.283	4493.625	482.892	4100.898	-46.566
4700	1162.420	3103.149	2122.334	4609.828	477.283	4179.549	-46.450
4800	1163.151	3127.630	2143.024	4726.107	471.315	4258.440	-46.340
4900	1163.839	3151.620	2163.363	4842.457	464.905	4337.311	-46.235
5000	1164.488	3175.139	2183.365	4958.874	458.156	4416.525	-46.138

3.454. Benzo[*b*]naphtho[2,1-*g*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-69-8
Point Group: C₁

Length: 15.88 Å
Width: 11.91 Å
Breadth: 5.774 Å
L/B Ratio: 1.333

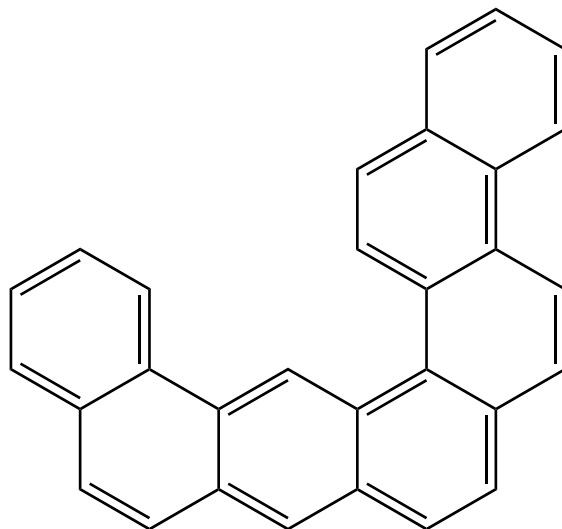
Cartesian coordinates:

C	-5.6250	2.3178	0.4143	C	2.1734	-3.5640	0.0357	H	-6.5929	-0.9493	0.0968
C	-6.4751	1.1802	0.3221	C	3.5259	-3.7998	0.0885	H	-3.6107	3.0505	0.4127
C	-5.9483	-0.0659	0.1661	C	4.4157	-2.7166	0.0885	H	-4.6003	-2.4014	-0.0597
C	-4.2721	2.1795	0.3420	C	3.9320	-1.4300	0.0613	H	-1.6682	1.6251	0.1435
C	-3.6847	0.8859	0.1703	C	0.6715	0.3498	-0.4099	H	-2.6802	-3.8434	-0.1421
C	-4.5315	-0.2460	0.0911	C	2.0198	0.1905	-0.0690	H	-0.2351	-4.1572	-0.0099
C	-3.9542	-1.5149	-0.0345	C	1.1042	2.6358	-1.1299	H	1.4771	-4.4153	0.0173
C	-2.2957	0.7245	0.0750	C	0.2661	1.5728	-1.0320	H	3.9123	-4.8236	0.1198
C	-1.7092	-0.5275	-0.1048	C	2.3773	2.5933	-0.4873	H	5.4949	-2.9009	0.1023
C	-2.5716	-1.6634	-0.1050	C	2.8241	1.3847	0.0848	H	4.6512	-0.5998	0.0421
C	-2.0037	-2.9812	-0.1168	C	4.0102	1.4326	0.8587	H	0.8067	3.5459	-1.6629
C	-0.6642	-3.1455	-0.0568	C	4.7417	2.5889	0.9784	H	-0.7411	1.6306	-1.4668
C	-0.2711	-0.7332	-0.2130	C	4.3290	3.7656	0.3272	H	4.3457	0.5290	1.3860
C	0.2306	-2.0217	-0.0810	C	3.1581	3.7692	-0.3882	H	5.6514	2.6039	1.5878
C	2.5445	-1.1549	0.0404	H	-6.0802	3.3051	0.5443	H	4.9367	4.6722	0.4104
C	1.6561	-2.2483	-0.0021	H	-7.5585	1.3268	0.3806	H	2.8056	4.6835	-0.8790

Table 3.454: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[2,1-*g*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.019	550.782	550.782	∞
100	125.766	373.198	866.631	-49.343	580.380	636.571	-332.504
200	246.789	495.505	650.544	-31.008	564.690	699.023	-182.562
250	317.078	558.067	625.763	-16.924	557.330	733.458	-153.245
298.15	385.741	619.799	619.799	0.000	550.782	767.990	-134.546
300	388.349	622.193	619.806	0.716	550.541	769.337	-133.951
350	456.969	687.262	624.788	21.866	544.520	806.293	-120.330
400	520.647	752.502	636.677	46.330	539.311	844.044	-110.219
450	578.348	817.217	653.149	73.830	534.822	882.410	-102.425
500	629.930	880.874	672.750	104.062	530.956	921.266	-96.242
600	716.441	1003.684	717.763	171.553	524.746	999.945	-87.051
700	784.891	1119.464	766.966	246.749	520.310	1079.526	-80.554
800	839.844	1227.988	817.885	328.082	517.436	1159.615	-75.714
900	884.684	1329.583	869.158	414.382	515.920	1239.975	-71.965
1000	921.778	1424.773	920.011	504.762	515.574	1320.455	-68.972
1100	952.797	1514.125	970.002	598.535	516.176	1400.931	-66.523
1200	978.957	1598.183	1018.883	695.159	517.568	1481.297	-64.478
1300	1001.176	1677.442	1066.522	794.196	519.546	1561.534	-62.742
1400	1020.165	1752.350	1112.860	895.287	521.961	1641.606	-61.248
1500	1036.485	1823.305	1157.878	998.140	524.722	1721.495	-59.947
1600	1050.585	1890.659	1201.590	1102.510	527.683	1801.182	-58.801
1700	1062.827	1954.726	1244.023	1208.195	530.762	1880.653	-57.784
1800	1073.507	2015.785	1285.216	1315.024	533.875	1960.013	-56.877
1900	1082.867	2074.083	1325.213	1422.853	536.985	2039.141	-56.059
2000	1091.106	2129.841	1364.061	1531.560	540.033	2118.135	-55.319
2100	1098.387	2183.256	1401.807	1641.042	542.931	2196.965	-54.645
2200	1104.849	2234.505	1438.500	1751.210	545.678	2275.664	-54.030
2300	1110.605	2283.747	1474.187	1861.988	548.267	2354.239	-53.465
2400	1115.750	2331.124	1508.911	1973.311	550.620	2432.654	-52.944
2500	1120.366	2376.767	1542.718	2085.120	552.750	2511.101	-52.466
2600	1124.520	2420.790	1575.649	2197.368	554.616	2589.339	-52.019
2700	1128.270	2463.302	1607.742	2310.011	556.223	2667.588	-51.607
2800	1131.666	2504.397	1639.036	2423.011	557.541	2745.810	-51.223
2900	1134.750	2544.163	1669.565	2536.334	558.539	2823.929	-50.863
3000	1137.558	2582.681	1699.364	2649.951	559.263	2902.048	-50.528
3100	1140.121	2620.024	1728.463	2763.837	559.629	2980.064	-50.213
3200	1142.466	2656.258	1756.893	2877.968	559.682	3058.154	-49.918
3300	1144.618	2691.447	1784.683	2992.324	559.402	3136.291	-49.642
3400	1146.596	2725.647	1811.857	3106.886	558.758	3214.347	-49.381
3500	1148.417	2758.911	1838.443	3221.638	557.755	3292.406	-49.135
3600	1150.099	2791.287	1864.463	3336.565	556.417	3370.595	-48.905
3700	1151.655	2822.820	1889.941	3451.654	554.709	3448.846	-48.688
3800	1153.096	2853.552	1914.896	3566.892	552.603	3527.080	-48.482
3900	1154.434	2883.522	1939.350	3682.269	550.143	3605.319	-48.287
4000	1155.678	2912.765	1963.321	3797.776	547.312	3683.778	-48.104
4100	1156.837	2941.316	1986.828	3913.402	544.069	3762.231	-47.930
4200	1157.917	2969.206	2009.887	4029.140	540.446	3840.758	-47.766
4300	1158.927	2996.465	2032.515	4144.983	536.427	3919.277	-47.609
4400	1159.872	3023.119	2054.727	4260.924	532.023	3997.995	-47.461
4500	1160.757	3049.195	2076.538	4376.956	527.247	4076.881	-47.322
4600	1161.587	3074.716	2097.961	4493.073	522.045	4155.885	-47.191
4700	1162.367	3099.706	2119.010	4609.271	516.431	4234.880	-47.064
4800	1163.100	3124.185	2139.697	4725.545	510.458	4314.116	-46.946
4900	1163.790	3148.175	2160.034	4841.890	504.043	4393.331	-46.833
5000	1164.441	3171.693	2180.033	4958.302	497.290	4472.890	-46.727

3.455. Phenanthro[2,3-*c*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-61-0
Point Group: C₁

Length: 16.26 Å
Width: 11.47 Å
Breadth: 5.242 Å
L/B Ratio: 1.418

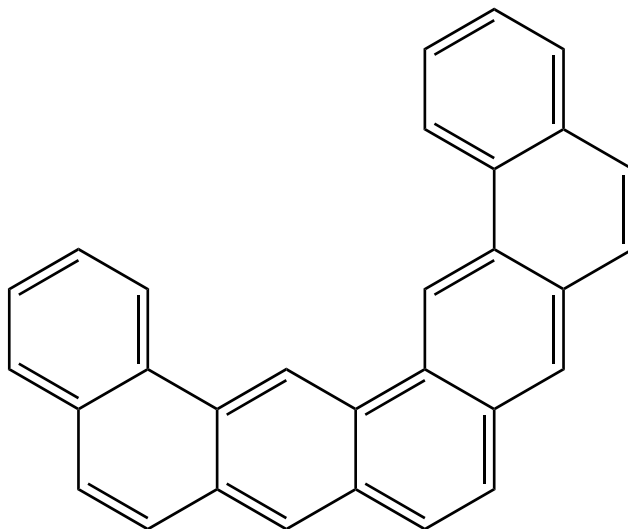
Cartesian coordinates:

C	-4.7898	3.5127	0.4146	C	0.8841	-1.4969	-0.0281	H	-1.5978	2.2978	0.4515
C	-5.4772	2.3387	0.1904	C	1.4467	-2.7629	0.1885	H	-2.8537	4.4395	0.6880
C	-2.6963	2.3189	0.3802	C	2.8295	-2.9057	0.4739	H	-6.5898	-0.0596	-0.2529
C	-3.3910	3.5024	0.5098	C	3.6438	-1.8130	0.4996	H	-5.3816	-2.2175	-0.4763
C	-3.3788	1.1076	0.1531	C	1.7823	-0.3851	-0.1889	H	-3.2934	-3.4828	-0.4022
C	-4.7812	1.1212	0.0569	C	3.1417	-0.5368	0.1346	H	-0.7352	0.7360	0.2665
C	-5.4973	-0.1067	-0.1780	C	2.2180	1.9222	-0.8669	H	-1.2881	-4.7852	-0.2485
C	-4.8403	-1.2808	-0.2998	C	1.3700	0.8707	-0.7486	H	1.1496	-4.9234	0.2169
C	-2.6662	-0.1494	0.0131	C	3.5747	1.8216	-0.4257	H	3.2286	-3.9046	0.6861
C	-3.4039	-1.3376	-0.1996	C	4.0433	0.5903	0.0624	H	4.7072	-1.9043	0.7683
C	-2.7255	-2.5515	-0.2812	C	5.3943	0.4926	0.4706	H	1.8824	2.8664	-1.3114
C	-1.2744	-0.2098	0.0795	C	6.2289	1.5822	0.4026	H	0.3397	0.9733	-1.1170
C	-0.5694	-1.4092	-0.0696	C	5.7512	2.8140	-0.0807	H	5.7632	-0.4747	0.8438
C	-1.3313	-2.6022	-0.1854	C	4.4451	2.9332	-0.4913	H	7.2723	1.4992	0.7238
C	-0.6792	-3.8814	-0.1321	H	-5.3317	4.4583	0.5190	H	6.4285	3.6730	-0.1277
C	0.6482	-3.9547	0.1064	H	-6.5706	2.3423	0.1146	H	4.0636	3.8874	-0.8719

Table 3.455: Table of thermodynamic data as a function of temperature for Phenanthro[2,3-*c*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.010	504.922	504.922	∞
100	125.409	377.725	870.118	-49.239	534.625	590.362	-308.367
200	246.286	499.654	654.447	-30.959	518.879	652.382	-170.381
250	316.593	562.108	629.705	-16.899	511.495	686.613	-143.457
298.15	385.184	623.749	623.749	0.000	504.922	720.953	-126.305
300	387.789	626.140	623.756	0.715	504.680	722.292	-125.760
350	456.306	691.115	628.731	21.834	498.628	759.053	-113.280
400	519.896	756.260	640.603	46.263	493.384	796.613	-104.025
450	577.541	820.883	657.051	73.724	488.856	834.794	-96.898
500	629.102	884.454	676.624	103.915	484.949	873.469	-91.249
600	715.648	1007.115	721.575	171.324	478.657	951.798	-82.860
700	784.190	1122.779	770.715	246.445	474.146	1031.042	-76.936
800	839.249	1231.217	821.574	327.714	471.208	1110.804	-72.527
900	884.192	1332.747	872.792	413.959	469.637	1190.845	-69.113
1000	921.376	1427.890	923.596	504.294	469.246	1271.010	-66.389
1100	952.469	1517.208	973.543	598.032	469.813	1351.177	-64.161
1200	978.690	1601.239	1022.384	694.626	471.175	1431.236	-62.299
1300	1000.958	1680.480	1069.989	793.638	473.128	1511.168	-60.718
1400	1019.986	1755.373	1116.295	894.710	475.524	1590.937	-59.357
1500	1036.337	1826.316	1161.286	997.546	478.268	1670.525	-58.172
1600	1050.462	1893.662	1204.972	1101.903	481.216	1749.911	-57.128
1700	1062.724	1957.722	1247.383	1207.577	484.284	1829.082	-56.200
1800	1073.421	2018.776	1288.556	1314.396	487.387	1908.142	-55.372
1900	1082.794	2077.069	1328.534	1422.217	490.490	1986.972	-54.625
2000	1091.043	2132.823	1367.365	1530.917	493.530	2065.668	-53.949
2100	1098.334	2186.235	1405.096	1640.393	496.422	2144.199	-53.333
2200	1104.802	2237.482	1441.775	1750.557	499.165	2222.600	-52.770
2300	1110.564	2286.722	1477.448	1861.330	501.749	2300.878	-52.254
2400	1115.715	2334.098	1512.161	1972.649	504.099	2378.996	-51.776
2500	1120.335	2379.739	1545.957	2084.456	506.226	2457.145	-51.338
2600	1124.493	2423.762	1578.877	2196.701	508.089	2535.085	-50.929
2700	1128.246	2466.272	1610.961	2309.341	509.693	2613.038	-50.551
2800	1131.645	2507.366	1642.246	2422.338	511.009	2690.962	-50.199
2900	1134.731	2547.132	1672.767	2535.659	512.004	2768.785	-49.870
3000	1137.541	2585.649	1702.557	2649.275	512.727	2846.607	-49.563
3100	1140.105	2622.991	1731.650	2763.159	513.091	2924.326	-49.274
3200	1142.452	2659.226	1760.073	2877.289	513.143	3002.119	-49.004
3300	1144.605	2694.414	1787.856	2991.643	512.861	3079.960	-48.751
3400	1146.584	2728.614	1815.025	3106.204	512.216	3157.719	-48.511
3500	1148.407	2761.877	1841.605	3220.955	511.212	3235.481	-48.286
3600	1150.090	2794.253	1867.619	3335.881	509.873	3313.373	-48.075
3700	1151.646	2825.786	1893.091	3450.968	508.164	3391.328	-47.876
3800	1153.088	2856.517	1918.042	3566.206	506.057	3469.265	-47.687
3900	1154.426	2886.487	1942.491	3681.583	503.597	3547.208	-47.509
4000	1155.671	2915.730	1966.458	3797.088	500.764	3625.371	-47.342
4100	1156.830	2944.281	1989.961	3912.714	497.521	3703.527	-47.183
4200	1157.911	2972.171	2013.016	4028.452	493.898	3781.758	-47.032
4300	1158.922	2999.429	2035.640	4144.294	489.878	3859.980	-46.888
4400	1159.867	3026.083	2057.848	4260.234	485.473	3938.402	-46.754
4500	1160.752	3052.159	2079.656	4376.265	480.697	4016.991	-46.627
4600	1161.582	3077.680	2101.075	4492.382	475.494	4095.698	-46.507
4700	1162.362	3102.670	2122.121	4608.580	469.880	4174.397	-46.392
4800	1163.096	3127.149	2142.805	4724.853	463.906	4253.337	-46.285
4900	1163.787	3151.139	2163.139	4841.198	457.491	4332.256	-46.181
5000	1164.438	3174.657	2183.135	4957.609	450.737	4411.518	-46.086

3.456. Dibenzo[*a,o*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-60-9
Point Group: C_{2v}

Length: 16.09 Å
Width: 11.63 Å
Breadth: 3.885 Å
L/B Ratio: 1.384

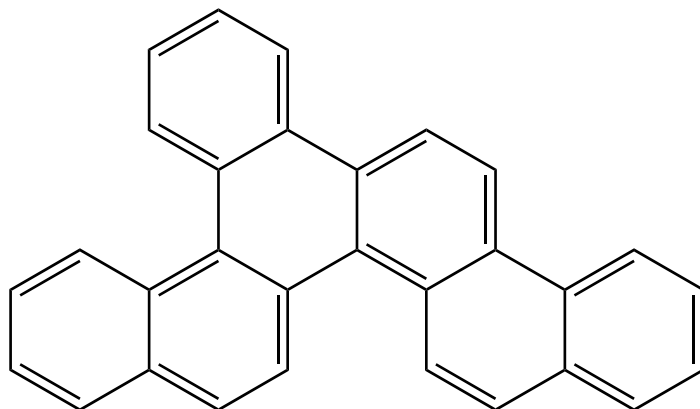
Cartesian coordinates:

C	5.1183	-3.4107	0.0000	C	-0.7319	1.3540	0.0000	H	1.8741	-2.3379	0.0000
C	5.7607	-2.1914	0.0000	C	-1.4304	2.5857	0.0000	H	3.2166	-4.4439	0.0000
C	2.9747	-2.3091	0.0000	C	-2.8243	2.5909	0.0000	H	6.7764	0.2927	0.0000
C	3.7167	-3.4699	0.0000	C	-1.4515	0.1612	0.0000	H	5.4766	2.4069	0.0000
C	3.6113	-1.0518	0.0000	C	-2.8494	0.1587	0.0000	H	3.3380	3.5712	0.0000
C	5.0157	-0.9949	0.0000	C	-3.5428	1.3906	0.0000	H	0.9139	-0.7963	0.0000
C	5.6803	0.2821	0.0000	C	-4.9830	1.3958	0.0000	H	1.2215	4.7713	0.0000
C	4.9722	1.4337	0.0000	C	-5.6823	0.2387	0.0000	H	-1.2579	4.7619	0.0000
C	2.8481	0.1804	0.0000	C	-3.6032	-1.0793	0.0000	H	-3.3651	3.5456	0.0000
C	3.5321	1.4176	0.0000	C	-5.0080	-1.0332	0.0000	H	-0.9078	-0.8033	0.0000
C	2.8044	2.6124	0.0000	C	-5.7438	-2.2353	0.0000	H	-5.4948	2.3651	0.0000
C	1.4503	0.1723	0.0000	C	-5.0922	-3.4497	0.0000	H	-6.7785	0.2410	0.0000
C	0.7216	1.3595	0.0000	C	-3.6901	-3.4982	0.0000	H	-6.8390	-2.1930	0.0000
C	1.4107	2.5965	0.0000	C	-2.9569	-2.3317	0.0000	H	-5.6646	-4.3831	0.0000
C	0.6600	3.8299	0.0000	H	5.6978	-4.3397	0.0000	H	-3.1826	-4.4683	0.0000
C	-0.6891	3.8247	0.0000	H	6.8555	-2.1407	0.0000	H	-1.8562	-2.3521	0.0000

Table 3.456: Table of thermodynamic data as a function of temperature for Dibenzo[*a,o*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.265	477.598	477.598	∞
100	126.495	376.364	870.262	-49.390	507.150	563.024	-294.088
200	246.987	498.928	654.028	-31.020	491.494	625.142	-163.267
250	317.210	561.527	629.239	-16.928	484.142	659.405	-137.772
298.15	385.765	623.273	623.273	0.000	477.598	693.771	-121.543
300	388.369	625.668	623.281	0.716	477.357	695.110	-121.027
350	456.853	690.730	628.263	21.864	471.334	731.893	-109.227
400	520.404	755.945	640.149	46.318	466.116	769.471	-100.481
450	578.007	820.626	656.617	73.804	461.612	807.666	-93.749
500	629.529	884.244	676.209	104.018	457.728	846.352	-88.416
600	716.013	1006.977	721.201	171.465	451.475	924.698	-80.500
700	784.518	1122.694	770.378	246.621	446.999	1003.953	-74.914
800	839.558	1231.174	821.272	327.922	444.092	1083.722	-70.758
900	884.489	1332.740	872.521	414.197	442.551	1163.765	-67.542
1000	921.663	1427.914	923.353	504.562	442.190	1243.930	-64.975
1100	952.747	1517.259	973.325	598.327	442.784	1324.092	-62.875
1200	978.957	1601.314	1022.190	694.949	444.174	1404.145	-61.120
1300	1001.213	1680.575	1069.816	793.987	446.153	1484.069	-59.629
1400	1020.228	1755.487	1116.142	895.083	448.574	1563.828	-58.346
1500	1036.566	1826.446	1161.151	997.943	451.342	1643.403	-57.227
1600	1050.678	1893.806	1204.855	1102.322	454.312	1722.775	-56.242
1700	1062.927	1957.879	1247.281	1208.017	457.400	1801.931	-55.365
1800	1073.612	2018.944	1288.468	1314.856	460.523	1880.975	-54.583
1900	1082.973	2077.247	1328.460	1422.695	463.644	1959.787	-53.877
2000	1091.211	2133.010	1367.304	1531.413	466.702	2038.465	-53.238
2100	1098.492	2186.431	1405.047	1640.906	469.611	2116.978	-52.656
2200	1104.951	2237.684	1441.737	1751.084	472.368	2195.359	-52.123
2300	1110.704	2286.931	1477.421	1861.872	474.967	2273.616	-51.634
2400	1115.846	2334.313	1512.144	1973.204	477.331	2351.712	-51.183
2500	1120.458	2379.959	1545.949	2085.024	479.470	2429.840	-50.768
2600	1124.609	2423.986	1578.878	2197.281	481.345	2507.758	-50.380
2700	1128.356	2466.501	1610.970	2309.932	482.960	2585.688	-50.022
2800	1131.748	2507.599	1642.263	2422.940	484.287	2663.589	-49.689
2900	1134.829	2547.368	1672.792	2536.271	485.292	2741.388	-49.377
3000	1137.633	2585.888	1702.590	2649.897	486.025	2819.187	-49.085
3100	1140.193	2623.234	1731.688	2763.790	486.398	2896.882	-48.811
3200	1142.536	2659.471	1760.118	2877.928	486.458	2974.651	-48.555
3300	1144.684	2694.662	1787.907	2992.291	486.185	3052.467	-48.316
3400	1146.659	2728.864	1815.082	3106.859	485.547	3130.201	-48.089
3500	1148.478	2762.129	1841.667	3221.617	484.550	3207.938	-47.875
3600	1150.158	2794.507	1867.687	3336.550	483.218	3285.805	-47.675
3700	1151.711	2826.041	1893.164	3451.645	481.517	3363.734	-47.486
3800	1153.150	2856.775	1918.120	3566.888	479.416	3441.646	-47.308
3900	1154.486	2886.746	1942.574	3682.271	476.961	3519.562	-47.138
4000	1155.728	2915.991	1966.545	3797.782	474.135	3597.700	-46.980
4100	1156.884	2944.543	1990.052	3913.414	470.897	3675.830	-46.830
4200	1157.963	2972.434	2013.111	4029.157	467.279	3754.034	-46.687
4300	1158.971	2999.694	2035.739	4145.004	463.264	3832.230	-46.551
4400	1159.914	3026.349	2057.951	4260.949	458.864	3910.626	-46.424
4500	1160.797	3052.425	2079.762	4376.985	454.093	3989.188	-46.304
4600	1161.626	3077.948	2101.185	4493.106	448.895	4067.869	-46.191
4700	1162.404	3102.938	2122.234	4609.308	443.285	4146.541	-46.083
4800	1163.136	3127.418	2142.921	4725.586	437.315	4225.454	-45.981
4900	1163.826	3151.409	2163.259	4841.934	430.903	4304.345	-45.884
5000	1164.475	3174.928	2183.258	4958.350	424.154	4383.580	-45.794

3.457. Naphtho[1,2-*f*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-49-4
Point Group: C₁

Length: 16.67 Å
Width: 11.61 Å
Breadth: 5.583 Å
L/B Ratio: 1.436

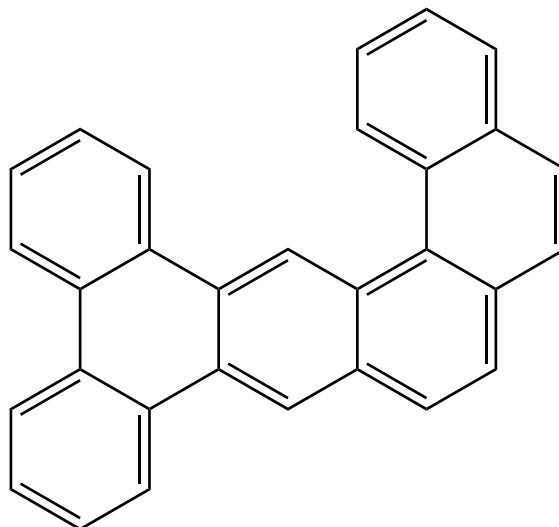
Cartesian coordinates:

C	6.4666	-0.2552	-0.5879	C	-3.3849	-2.0043	0.8203	H	5.8403	2.6502	1.0839
C	6.7080	0.9729	0.0542	C	-3.4709	-3.3794	0.8787	H	4.9886	-1.7035	-1.1929
C	5.6623	1.6937	0.5795	C	-2.4241	-4.1703	0.3904	H	3.4524	2.8595	1.5821
C	5.1859	-0.7418	-0.6954	C	-1.2742	-3.5657	-0.0671	H	1.1404	2.0682	1.3186
C	4.0917	-0.0166	-0.1692	C	-2.1559	0.0783	0.0907	H	1.0428	-3.3689	-1.0484
C	4.3394	1.2077	0.4741	C	-0.8793	0.6486	0.0347	H	3.3382	-2.3854	-1.1774
C	3.2405	1.9376	1.0281	C	-0.7581	2.0630	-0.1078	H	-4.2161	-1.4001	1.2085
C	1.9675	1.4962	0.8759	C	-1.8449	2.8766	-0.1575	H	-4.3590	-3.8573	1.3051
C	2.7355	-0.5038	-0.2732	C	-3.3148	0.9194	-0.0953	H	-2.5134	-5.2613	0.3974
C	1.6601	0.2835	0.1720	C	-3.1527	2.3195	-0.1622	H	-0.4231	-4.1717	-0.4137
C	1.2322	-2.3278	-0.7458	C	-4.2753	3.1762	-0.2937	H	0.2428	2.5099	-0.1814
C	2.4898	-1.8017	-0.7893	C	-5.5352	2.6549	-0.4198	H	-1.7297	3.9642	-0.2324
C	0.1362	-1.5426	-0.3065	C	-5.7065	1.2567	-0.4401	H	-4.1151	4.2605	-0.3032
C	0.3139	-0.1873	-0.0075	C	-4.6315	0.4200	-0.2859	H	-6.4070	3.3091	-0.5205
C	-1.1513	-2.1614	-0.0748	H	7.3085	-0.8202	-1.0013	H	-6.7099	0.8429	-0.5861
C	-2.2543	-1.3619	0.2762	H	7.7341	1.3469	0.1318	H	-4.8002	-0.6648	-0.3213

Table 3.457: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*f*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.929	538.906	538.906	∞
100	125.690	372.200	864.947	-49.275	568.573	624.863	-326.388
200	246.408	494.342	649.165	-30.965	552.857	687.422	-179.533
250	316.630	556.811	624.418	-16.902	545.476	721.918	-150.833
298.15	385.278	618.461	618.461	0.000	538.906	756.513	-132.535
300	387.887	620.853	618.469	0.715	538.664	757.862	-131.953
350	456.537	685.853	623.445	21.843	532.620	794.887	-118.628
400	520.264	751.038	635.322	46.286	527.391	832.709	-108.738
450	578.019	815.711	651.780	73.769	522.885	871.150	-101.118
500	629.649	879.336	671.365	103.986	519.003	910.082	-95.074
600	716.230	1002.102	716.349	171.452	512.768	988.917	-86.091
700	784.720	1117.853	765.525	246.629	508.314	1068.658	-79.743
800	839.691	1226.355	816.422	327.946	505.424	1148.910	-75.015
900	884.541	1327.932	867.675	414.231	503.893	1229.434	-71.353
1000	921.641	1423.108	918.511	504.597	503.533	1310.079	-68.430
1100	952.664	1512.447	968.486	598.357	504.122	1390.723	-66.039
1200	978.829	1596.493	1017.353	694.968	505.501	1471.257	-64.041
1300	1001.053	1675.743	1064.980	793.992	507.466	1551.664	-62.345
1400	1020.048	1750.642	1111.305	895.072	509.869	1631.906	-60.886
1500	1036.373	1821.589	1156.314	997.913	512.619	1711.967	-59.615
1600	1050.479	1888.936	1200.016	1102.272	515.569	1791.825	-58.496
1700	1062.727	1952.997	1242.440	1207.947	518.638	1871.469	-57.502
1800	1073.413	2014.050	1283.625	1314.766	521.741	1951.002	-56.615
1900	1082.778	2072.343	1323.614	1422.585	524.842	2030.304	-55.816
2000	1091.022	2128.096	1362.454	1531.284	527.881	2109.473	-55.093
2100	1098.309	2181.507	1400.194	1640.758	530.771	2188.477	-54.434
2200	1104.775	2232.753	1436.881	1750.918	533.510	2267.351	-53.833
2300	1110.535	2281.991	1472.561	1861.689	536.092	2346.102	-53.281
2400	1115.684	2329.366	1507.281	1973.005	538.439	2424.692	-52.771
2500	1120.304	2375.006	1541.082	2084.809	540.562	2503.315	-52.303
2600	1124.461	2419.027	1574.008	2197.050	542.422	2581.728	-51.866
2700	1128.215	2461.537	1606.097	2309.687	544.023	2660.155	-51.463
2800	1131.614	2502.630	1637.386	2422.682	545.336	2738.553	-51.087
2900	1134.701	2542.394	1667.911	2536.000	546.329	2816.849	-50.736
3000	1137.511	2580.910	1697.706	2649.613	547.048	2895.145	-50.408
3100	1140.077	2618.252	1726.802	2763.494	547.410	2973.338	-50.099
3200	1142.424	2654.485	1755.229	2877.621	547.458	3051.605	-49.811
3300	1144.578	2689.673	1783.015	2991.972	547.174	3129.920	-49.541
3400	1146.558	2723.872	1810.186	3106.530	546.526	3208.153	-49.286
3500	1148.381	2757.134	1836.769	3221.279	545.519	3286.390	-49.046
3600	1150.065	2789.509	1862.786	3336.202	544.178	3364.756	-48.820
3700	1151.622	2821.041	1888.261	3451.287	542.467	3443.185	-48.608
3800	1153.065	2851.772	1913.214	3566.523	540.357	3521.597	-48.407
3900	1154.404	2881.741	1937.665	3681.897	537.895	3600.014	-48.216
4000	1155.649	2910.984	1961.634	3797.400	535.060	3678.652	-48.037
4100	1156.809	2939.534	1985.138	3913.024	531.815	3757.283	-47.867
4200	1157.891	2967.424	2008.195	4028.759	528.189	3835.988	-47.707
4300	1158.902	2994.682	2030.821	4144.600	524.168	3914.685	-47.553
4400	1159.848	3021.335	2053.031	4260.538	519.761	3993.582	-47.409
4500	1160.734	3047.410	2074.840	4376.567	514.983	4072.646	-47.273
4600	1161.565	3072.931	2096.261	4492.683	509.778	4151.828	-47.145
4700	1162.345	3097.920	2117.308	4608.878	504.162	4231.002	-47.021
4800	1163.079	3122.400	2137.993	4725.150	498.187	4310.416	-46.906
4900	1163.771	3146.389	2158.329	4841.493	491.770	4389.810	-46.795
5000	1164.422	3169.907	2178.326	4957.903	485.015	4469.547	-46.692

3.458. Phenanthro[3,4-*b*]triphenylene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 112498-95-0
Point Group: C₁

Length: 15.68 Å
Width: 11.07 Å
Breadth: 5.253 Å
L/B Ratio: 1.417

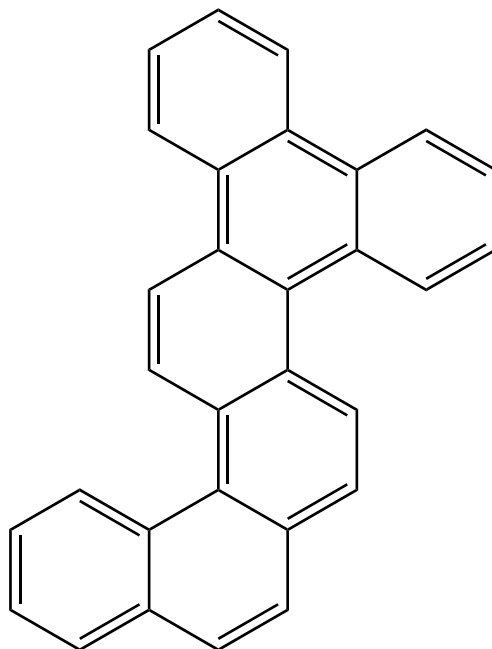
Cartesian coordinates:

C	-3.4699	3.7149	-0.4302	C	1.1478	-0.8390	-0.0183	H	-0.2039	2.7501	-0.4333
C	-4.0654	2.4798	-0.2580	C	0.5090	-2.1010	0.0362	H	-1.6054	4.7912	-0.6304
C	-1.3013	2.6755	-0.3851	C	1.2814	-3.3046	-0.0417	H	-5.9356	0.8130	0.0365
C	-2.0782	3.8132	-0.4940	C	2.6185	-3.2367	-0.2425	H	-7.0186	-1.4040	0.3469
C	-1.8899	1.4111	-0.2121	C	2.5982	-0.7795	-0.0295	H	-5.6242	-3.4584	0.5178
C	-3.2904	1.3129	-0.1467	C	3.2912	-1.9717	-0.2638	H	-3.1441	-3.2931	0.3781
C	-3.1394	-1.1453	0.1332	C	4.6955	-1.9702	-0.5272	H	-1.3702	-3.1748	0.1867
C	-3.9257	0.0144	0.0353	C	5.3999	-0.8111	-0.5070	H	0.7744	1.2865	-0.2841
C	-5.3241	-0.0989	0.1144	C	3.3800	0.4198	0.1838	H	0.7643	-4.2685	0.0264
C	-5.9280	-1.3301	0.2863	C	4.7609	0.4035	-0.1116	H	3.2155	-4.1473	-0.3700
C	-5.1455	-2.4832	0.3824	C	5.5413	1.5761	0.0340	H	5.1858	-2.9218	-0.7640
C	-3.7689	-2.3896	0.3059	C	4.9842	2.7271	0.5300	H	6.4675	-0.7915	-0.7542
C	-1.0663	0.2130	-0.0977	C	3.6322	2.7301	0.9176	H	6.6016	1.5453	-0.2429
C	-1.6879	-1.0514	0.0558	C	2.8570	1.6093	0.7507	H	5.5834	3.6361	0.6435
C	-0.8908	-2.1855	0.1049	H	-4.0859	4.6158	-0.5165	H	3.2036	3.6345	1.3623
C	0.3200	0.2910	-0.1371	H	-5.1617	2.3954	-0.2056	H	1.8108	1.6371	1.0850

Table 3.458: Table of thermodynamic data as a function of temperature for Phenanthro[3,4-*b*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.099	507.716	507.716	∞
100	126.607	378.254	870.719	-49.247	537.412	593.097	-309.796
200	246.202	500.631	655.175	-30.909	521.724	655.031	-171.073
250	316.041	563.011	630.476	-16.866	514.322	689.214	-144.000
298.15	384.404	624.532	624.532	0.000	507.716	723.514	-126.754
300	387.004	626.918	624.539	0.714	507.473	724.851	-126.205
350	455.453	691.765	629.504	21.791	501.380	761.577	-113.657
400	519.064	756.797	641.353	46.177	496.093	799.108	-104.351
450	576.769	821.326	657.773	73.599	491.525	837.264	-97.185
500	628.397	884.819	677.313	103.753	487.581	875.918	-91.505
600	715.057	1007.362	722.200	171.097	481.224	954.217	-83.070
700	783.673	1122.941	771.279	246.163	476.659	1033.441	-77.115
800	838.776	1231.312	822.084	327.383	473.671	1113.191	-72.682
900	883.747	1332.789	873.253	413.582	472.054	1193.225	-69.252
1000	920.952	1427.886	924.013	503.874	471.620	1273.388	-66.514
1100	952.065	1517.165	973.919	597.570	472.145	1353.557	-64.274
1200	978.306	1601.162	1022.725	694.125	473.468	1433.622	-62.403
1300	1000.593	1680.372	1070.295	793.099	475.384	1513.564	-60.814
1400	1019.641	1755.239	1116.571	894.136	477.744	1593.345	-59.447
1500	1036.012	1826.159	1161.534	996.939	480.455	1672.947	-58.256
1600	1050.156	1893.484	1205.195	1101.264	483.371	1752.350	-57.207
1700	1062.437	1957.527	1247.581	1206.908	486.409	1831.539	-56.275
1800	1073.152	2018.564	1288.731	1313.699	489.485	1910.620	-55.444
1900	1082.542	2076.844	1328.689	1421.494	492.561	1989.471	-54.693
2000	1090.807	2132.585	1367.500	1530.170	495.578	2068.191	-54.014
2100	1098.112	2185.986	1405.213	1639.623	498.447	2146.747	-53.396
2200	1104.595	2237.223	1441.875	1749.765	501.168	2225.173	-52.831
2300	1110.369	2286.454	1477.533	1860.519	503.732	2303.477	-52.313
2400	1115.531	2333.822	1512.231	1971.819	506.063	2381.622	-51.834
2500	1120.162	2379.456	1546.013	2083.607	508.172	2459.799	-51.394
2600	1124.330	2423.472	1578.920	2195.836	510.018	2537.768	-50.983
2700	1128.093	2465.976	1610.991	2308.460	511.606	2615.750	-50.604
2800	1131.500	2507.065	1642.264	2421.442	512.908	2693.704	-50.251
2900	1134.594	2546.826	1672.774	2534.749	513.889	2771.557	-49.920
3000	1137.411	2585.338	1702.555	2648.352	514.598	2849.410	-49.612
3100	1139.983	2622.677	1731.637	2762.224	514.950	2927.161	-49.321
3200	1142.336	2658.907	1760.051	2876.341	514.990	3004.986	-49.050
3300	1144.495	2694.092	1787.824	2990.684	514.697	3082.858	-48.797
3400	1146.479	2728.289	1814.985	3105.234	514.041	3160.649	-48.556
3500	1148.307	2761.549	1841.556	3219.975	513.026	3238.444	-48.330
3600	1149.995	2793.922	1867.563	3334.891	511.678	3316.370	-48.118
3700	1151.556	2825.452	1893.028	3449.970	509.960	3394.357	-47.919
3800	1153.002	2856.182	1917.971	3565.199	507.844	3472.328	-47.729
3900	1154.344	2886.149	1942.414	3680.567	505.375	3550.304	-47.550
4000	1155.593	2915.390	1966.374	3796.064	502.535	3628.501	-47.382
4100	1156.755	2943.939	1989.871	3911.682	499.284	3706.692	-47.223
4200	1157.840	2971.827	2012.920	4027.413	495.653	3784.957	-47.072
4300	1158.853	2999.084	2035.538	4143.248	491.626	3863.213	-46.928
4400	1159.800	3025.736	2057.741	4259.181	487.214	3941.670	-46.793
4500	1160.688	3051.811	2079.543	4375.206	482.432	4020.294	-46.665
4600	1161.521	3077.330	2100.957	4491.317	477.223	4099.036	-46.545
4700	1162.304	3102.319	2121.998	4607.508	471.603	4177.770	-46.430
4800	1163.040	3126.797	2142.677	4723.776	465.623	4256.745	-46.322
4900	1163.732	3150.785	2163.007	4840.115	459.202	4335.699	-46.218
5000	1164.385	3174.302	2182.998	4956.521	452.444	4414.996	-46.122

3.459. Dibenzo[*a,j*]plcencene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-54-1
Point Group: C_1

Length: 16.25 Å
Width: 10.84 Å
Breadth: 6.020 Å
L/B Ratio: 1.499

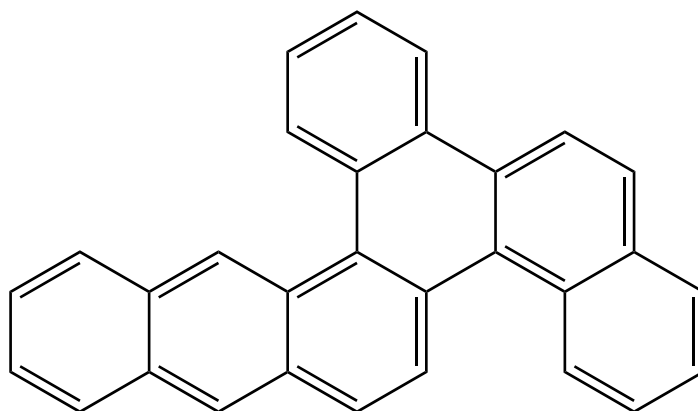
Cartesian coordinates:

C	-6.0557	1.8517	-0.9452	C	1.4734	1.0357	0.1364	H	-2.6731	1.9680	-1.2876
C	-6.1756	0.6863	-0.2301	C	1.2116	-0.3320	0.0368	H	-4.6906	3.2065	-1.9382
C	-3.6561	1.6025	-0.9608	C	2.8353	1.5352	0.2036	H	-6.2034	-1.6554	1.0353
C	-4.7807	2.2987	-1.3324	C	3.9096	0.6390	0.0986	H	-4.2248	-3.1018	1.4601
C	-3.7367	0.4241	-0.1789	C	5.2257	1.1178	0.2493	H	-1.8915	-3.5146	1.3421
C	-5.0269	-0.0550	0.1345	C	5.4690	2.4554	0.4781	H	0.4051	-2.8243	0.7920
C	-5.1916	-1.3220	0.7776	C	4.3995	3.3556	0.5559	H	0.6135	3.0255	0.2902
C	-4.1118	-2.1041	1.0202	C	3.1047	2.9013	0.4207	H	-1.7150	2.2571	0.1870
C	-2.5778	-0.3401	0.2363	C	3.6446	-0.7533	-0.2117	H	6.0606	0.4048	0.1736
C	-2.7936	-1.6328	0.7258	C	2.3189	-1.2238	-0.2889	H	6.4952	2.8181	0.5954
C	-1.6934	-2.5095	0.9515	C	2.1159	-2.5336	-0.7691	H	4.5956	4.4190	0.7274
C	-0.4255	-2.1171	0.6628	C	3.1727	-3.3657	-1.0750	H	2.2630	3.6069	0.4879
C	-1.2131	0.1336	0.1793	C	4.4871	-2.9171	-0.9148	H	1.0918	-2.9072	-0.9059
C	-0.1399	-0.7802	0.2501	C	4.7145	-1.6233	-0.4978	H	2.9847	-4.3788	-1.4456
C	0.3911	1.9502	0.2129	H	-6.9423	2.4277	-1.2289	H	5.3256	-3.5854	-1.1351
C	-0.9012	1.5192	0.1740	H	-7.1641	0.3099	0.0577	H	5.7439	-1.2473	-0.3940

Table 3.459: Table of thermodynamic data as a function of temperature for Dibenzo[*a,j*]plcene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.027	531.583	531.583	∞
100	125.954	374.982	867.915	-49.293	561.232	617.244	-322.409
200	246.529	497.261	652.081	-30.964	545.535	679.516	-177.468
250	316.620	559.743	627.337	-16.898	538.157	713.866	-149.151
298.15	385.149	621.382	621.382	0.000	531.583	748.320	-131.100
300	387.754	623.772	621.389	0.715	531.341	749.663	-130.525
350	456.316	688.745	626.364	21.833	525.288	786.543	-117.383
400	519.990	753.896	638.235	46.264	520.046	824.222	-107.630
450	577.718	818.535	654.685	73.733	515.526	862.520	-100.117
500	629.340	882.128	674.260	103.934	511.629	901.311	-94.157
600	715.932	1004.838	719.222	171.370	505.364	979.871	-85.304
700	784.449	1120.545	768.376	246.519	500.881	1059.340	-79.047
800	839.449	1229.013	819.250	327.810	497.965	1139.324	-74.389
900	884.326	1330.563	870.483	414.072	496.411	1219.584	-70.781
1000	921.451	1425.718	921.300	504.418	496.031	1299.967	-67.902
1100	952.495	1515.040	971.258	598.160	496.602	1380.351	-65.546
1200	978.678	1599.072	1020.110	694.755	497.965	1460.627	-63.578
1300	1000.918	1678.310	1067.722	793.764	499.916	1540.776	-61.908
1400	1019.926	1753.200	1114.035	894.831	502.306	1620.762	-60.470
1500	1036.263	1824.138	1159.031	997.661	505.044	1700.567	-59.218
1600	1050.379	1891.479	1202.723	1102.010	507.984	1780.171	-58.115
1700	1062.636	1955.534	1245.137	1207.675	511.043	1859.561	-57.136
1800	1073.330	2016.582	1286.313	1314.485	514.137	1938.840	-56.263
1900	1082.702	2074.871	1326.294	1422.297	517.231	2017.889	-55.474
2000	1090.952	2130.620	1365.126	1530.988	520.262	2096.806	-54.762
2100	1098.244	2184.028	1402.859	1640.455	523.145	2175.558	-54.113
2200	1104.715	2235.271	1439.539	1750.609	525.878	2254.180	-53.520
2300	1110.480	2284.507	1475.213	1861.375	528.455	2332.679	-52.976
2400	1115.633	2331.879	1509.927	1972.685	530.796	2411.018	-52.473
2500	1120.256	2377.517	1543.724	2084.484	532.915	2489.390	-52.012
2600	1124.417	2421.537	1576.644	2196.721	534.770	2567.552	-51.582
2700	1128.173	2464.044	1608.728	2309.353	536.367	2645.727	-51.184
2800	1131.575	2505.136	1640.013	2422.344	537.676	2723.875	-50.813
2900	1134.664	2544.899	1670.534	2535.658	538.664	2801.920	-50.467
3000	1137.477	2583.414	1700.325	2649.267	539.380	2879.966	-50.144
3100	1140.044	2620.754	1729.417	2763.145	539.738	2957.909	-49.839
3200	1142.394	2656.987	1757.840	2877.269	539.784	3035.926	-49.555
3300	1144.549	2692.173	1785.623	2991.618	539.497	3113.990	-49.289
3400	1146.530	2726.372	1812.791	3106.173	538.846	3191.973	-49.038
3500	1148.356	2759.633	1839.371	3220.918	537.837	3269.960	-48.800
3600	1150.040	2792.007	1865.385	3335.839	536.492	3348.077	-48.578
3700	1151.599	2823.539	1890.857	3450.922	534.779	3426.256	-48.369
3800	1153.043	2854.269	1915.807	3566.155	532.667	3504.418	-48.171
3900	1154.383	2884.238	1940.256	3681.527	530.203	3582.585	-47.982
4000	1155.629	2913.480	1964.223	3797.029	527.366	3660.973	-47.806
4100	1156.790	2942.030	1987.725	3912.650	524.119	3739.355	-47.639
4200	1157.873	2969.919	2010.780	4028.384	520.491	3817.810	-47.480
4300	1158.885	2997.176	2033.404	4144.223	516.468	3896.258	-47.329
4400	1159.831	3023.830	2055.612	4260.159	512.059	3974.905	-47.187
4500	1160.718	3049.904	2077.418	4376.187	507.280	4053.720	-47.053
4600	1161.549	3075.425	2098.838	4492.301	502.074	4132.653	-46.927
4700	1162.331	3100.414	2119.883	4608.495	496.456	4211.577	-46.805
4800	1163.065	3124.893	2140.566	4724.765	490.479	4290.742	-46.692
4900	1163.757	3148.881	2160.900	4841.107	484.061	4369.887	-46.583
5000	1164.409	3172.399	2180.896	4957.515	477.304	4449.375	-46.481

3.460. Tribenzo[*b,g,l*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-47-2
Point Group: C₁

Length: 16.37 Å
Width: 11.64 Å
Breadth: 5.912 Å
L/B Ratio: 1.405

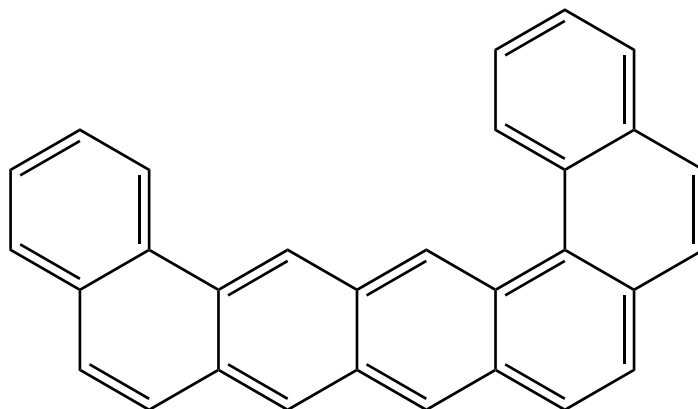
Cartesian coordinates:

C	-6.2981	-0.0208	1.1214	C	1.6243	3.6260	-0.1051	H	-5.6894	-2.8602	-0.6882
C	-6.5346	-1.2563	0.4576	C	0.6203	4.5595	-0.1969	H	-4.8643	1.4873	1.6364
C	-5.5191	-1.9063	-0.1766	C	-0.7108	4.1333	-0.3070	H	-3.2899	-2.9932	-1.2607
C	-5.0546	0.5359	1.1267	C	-1.0055	2.7906	-0.3006	H	-2.5315	1.4138	0.9517
C	-3.9681	-0.1144	0.4622	C	2.4149	1.2736	-0.0246	H	-0.9280	-3.1327	-1.8313
C	-4.2017	-1.3518	-0.1848	C	2.1430	-0.0907	-0.1285	H	1.3788	-2.3633	-1.4019
C	-3.1266	-2.0144	-0.7926	C	4.7902	0.8493	0.2455	H	2.6701	3.9600	-0.0345
C	-2.6850	0.4534	0.4378	C	3.7601	1.7260	0.1417	H	0.8523	5.6294	-0.1935
C	-1.6231	-0.1678	-0.2134	C	4.5320	-0.5528	0.2781	H	-1.5111	4.8740	-0.4055
C	-1.8541	-1.4542	-0.7831	C	3.2125	-1.0304	0.1320	H	-2.0548	2.4817	-0.4044
C	-0.7368	-2.1967	-1.2945	C	3.0056	-2.4204	0.3263	H	5.8244	1.2005	0.3371
C	0.5226	-1.7608	-1.0691	C	4.0488	-3.2769	0.5744	H	3.9536	2.8086	0.1706
C	-0.2775	0.3889	-0.2585	C	5.3686	-2.7940	0.6447	H	1.9856	-2.8256	0.2814
C	0.7877	-0.4898	-0.4502	C	5.6039	-1.4505	0.5063	H	3.8601	-4.3452	0.7244
C	0.0039	1.8066	-0.1798	H	-7.1340	0.4735	1.6271	H	6.1925	-3.4925	0.8222
C	1.3428	2.2403	-0.1051	H	-7.5465	-1.6744	0.4678	H	6.6222	-1.0518	0.5809

Table 3.460: Table of thermodynamic data as a function of temperature for Tribenzo[*b,g,l*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.127	550.257	550.257	∞
100	126.012	375.266	869.234	-49.397	579.802	635.786	-332.094
200	247.065	497.744	652.925	-31.036	564.137	698.022	-182.301
250	317.373	560.369	628.123	-16.938	556.791	732.343	-153.012
298.15	386.040	622.153	622.153	0.000	550.257	766.764	-134.331
300	388.648	624.549	622.161	0.717	550.017	768.106	-133.736
350	457.262	689.665	627.147	21.881	544.010	804.943	-120.129
400	520.927	754.942	639.043	46.360	538.816	842.572	-110.026
450	578.611	819.690	655.526	73.874	534.341	880.816	-102.240
500	630.176	883.374	675.137	104.118	530.488	919.547	-96.062
600	716.652	1006.226	720.173	171.632	524.300	997.974	-86.880
700	785.073	1122.036	769.397	246.848	519.884	1077.299	-80.387
800	840.001	1230.583	820.335	328.198	517.027	1157.131	-75.551
900	884.821	1332.194	871.625	414.512	515.525	1237.230	-71.806
1000	921.899	1427.398	922.493	504.905	515.192	1317.448	-68.815
1100	952.904	1516.761	972.498	598.690	515.806	1397.661	-66.368
1200	979.052	1600.828	1021.391	695.324	517.208	1477.763	-64.324
1300	1001.262	1680.094	1069.041	794.369	519.194	1557.735	-62.589
1400	1020.242	1755.008	1115.388	895.469	521.618	1637.542	-61.096
1500	1036.554	1825.968	1160.415	998.329	524.386	1717.165	-59.796
1600	1050.648	1893.326	1204.135	1102.706	527.354	1796.585	-58.651
1700	1062.884	1957.397	1246.576	1208.396	530.439	1875.789	-57.635
1800	1073.560	2018.459	1287.775	1315.231	533.557	1954.882	-56.728
1900	1082.915	2076.760	1327.778	1423.064	536.673	2033.742	-55.910
2000	1091.150	2132.520	1366.632	1531.776	539.725	2112.469	-55.171
2100	1098.428	2185.937	1404.383	1641.263	542.627	2191.031	-54.498
2200	1104.887	2237.188	1441.081	1751.435	545.378	2269.461	-53.883
2300	1110.640	2286.431	1476.772	1862.216	547.971	2347.768	-53.318
2400	1115.782	2333.810	1511.501	1973.542	550.327	2425.915	-52.798
2500	1120.396	2379.454	1545.312	2085.355	552.460	2504.093	-52.319
2600	1124.548	2423.479	1578.246	2197.606	554.329	2582.062	-51.873
2700	1128.297	2465.991	1610.343	2310.251	555.939	2660.043	-51.461
2800	1131.691	2507.087	1641.639	2423.254	557.260	2737.995	-51.077
2900	1134.773	2546.854	1672.172	2536.579	558.259	2815.845	-50.718
3000	1137.580	2585.373	1701.973	2650.199	558.986	2893.695	-50.383
3100	1140.141	2622.716	1731.075	2764.087	559.354	2971.442	-50.067
3200	1142.486	2658.952	1759.508	2878.220	559.409	3049.263	-49.773
3300	1144.636	2694.141	1787.300	2992.578	559.131	3127.130	-49.497
3400	1146.613	2728.342	1814.477	3107.141	558.489	3204.916	-49.237
3500	1148.434	2761.606	1841.065	3221.895	557.487	3282.706	-48.991
3600	1150.115	2793.982	1867.087	3336.824	556.151	3360.625	-48.760
3700	1151.670	2825.516	1892.566	3451.914	554.445	3438.607	-48.543
3800	1153.110	2856.248	1917.523	3567.154	552.340	3516.571	-48.338
3900	1154.447	2886.218	1941.979	3682.532	549.882	3594.540	-48.142
4000	1155.691	2915.462	1965.952	3798.040	547.051	3672.731	-47.960
4100	1156.849	2944.014	1989.461	3913.668	543.810	3750.913	-47.786
4200	1157.929	2971.904	2012.521	4029.407	540.188	3829.171	-47.622
4300	1158.938	2999.163	2035.151	4145.251	536.170	3907.420	-47.465
4400	1159.882	3025.817	2057.364	4261.193	531.767	3985.868	-47.317
4500	1160.767	3051.893	2079.176	4377.226	526.993	4064.484	-47.178
4600	1161.597	3077.414	2100.600	4493.344	521.791	4143.218	-47.047
4700	1162.376	3102.404	2121.650	4609.543	516.179	4221.944	-46.921
4800	1163.109	3126.884	2142.339	4725.818	510.206	4300.910	-46.802
4900	1163.799	3150.874	2162.677	4842.164	503.792	4379.855	-46.689
5000	1164.449	3174.392	2182.677	4958.576	497.040	4459.143	-46.583

3.461. Benzo[*a*]naphtho[2,1-*l*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-87-0
Point Group: C₁

Length: 16.81 Å
Width: 11.18 Å
Breadth: 5.110 Å
L/B Ratio: 1.504

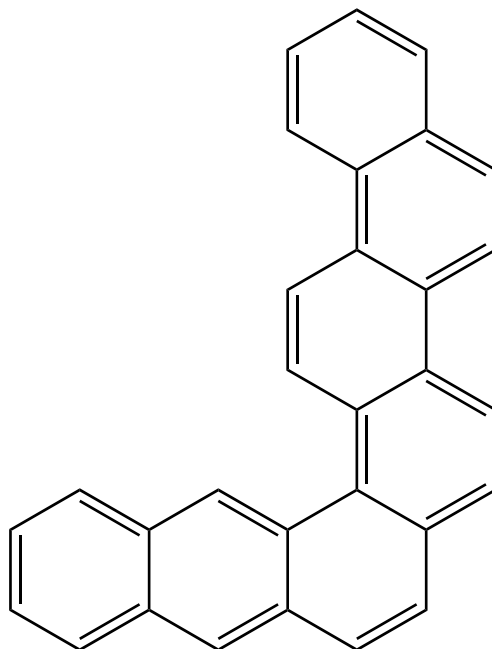
Cartesian coordinates:

C	-6.4128	2.3959	0.3357	C	1.8023	-0.8775	-0.0143	H	-3.0022	2.5083	0.4545
C	-6.5864	1.0434	0.1144	C	1.5640	-2.2869	-0.1244	H	-4.9943	4.0006	0.6345
C	-4.0213	2.1030	0.3593	C	2.6702	-3.2062	-0.0414	H	-6.6754	-1.6003	-0.3110
C	-5.1245	2.9278	0.4588	C	3.9134	-2.7520	0.2164	H	-4.7277	-3.1233	-0.4937
C	-4.1770	0.7241	0.1341	C	3.1810	-0.3999	0.0408	H	-2.3213	-3.4840	-0.4659
C	-5.4720	0.1928	0.0113	C	4.1833	-1.3394	0.2856	H	-1.5745	1.4017	0.3104
C	-5.6507	-1.2220	-0.2196	C	5.5157	-0.9351	0.5913	H	0.1125	-3.8644	-0.3427
C	-4.5915	-2.0496	-0.3189	C	5.8527	0.3812	0.5991	H	0.8287	1.0296	0.2902
C	-3.0230	-0.1570	0.0272	C	3.5801	0.9766	-0.1374	H	2.4666	-4.2774	-0.1534
C	-3.2383	-1.5537	-0.1988	C	4.8987	1.3603	0.1945	H	4.7524	-3.4454	0.3477
C	-2.1624	-2.4117	-0.2973	C	5.3037	2.7143	0.0812	H	6.2567	-1.7052	0.8360
C	-1.7350	0.3252	0.1370	C	4.4448	3.6589	-0.4159	H	6.8616	0.7060	0.8782
C	-0.6200	-0.5406	0.0276	C	3.1580	3.2727	-0.8378	H	6.3197	2.9899	0.3869
C	-0.8382	-1.9246	-0.1805	C	2.7421	1.9728	-0.7031	H	4.7519	4.7058	-0.5048
C	0.2770	-2.7848	-0.2346	H	-7.2823	3.0565	0.4158	H	2.4932	4.0210	-1.2822
C	0.6998	-0.0482	0.1134	H	-7.5943	0.6238	0.0177	H	1.7404	1.6974	-1.0604

Table 3.461: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[2,1-*l*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.998	519.703	519.703	∞
100	125.174	375.396	868.434	-49.304	549.342	605.312	-316.176
200	246.646	497.338	652.427	-31.018	533.602	667.568	-174.347
250	317.217	559.902	627.636	-16.933	526.242	701.911	-146.653
298.15	385.966	621.668	621.668	0.000	519.703	736.355	-129.004
300	388.575	624.063	621.675	0.716	519.463	737.697	-128.442
350	457.161	689.166	626.660	21.877	513.452	774.559	-115.594
400	520.757	754.426	638.554	46.349	508.251	812.214	-106.062
450	578.373	819.149	655.032	73.853	503.766	850.484	-98.720
500	629.890	882.806	674.638	104.084	499.899	889.243	-92.897
600	716.339	1005.601	719.657	171.567	493.681	967.730	-84.247
700	784.797	1121.366	768.862	246.753	489.235	1047.120	-78.135
800	839.791	1229.880	819.781	328.079	486.354	1127.020	-73.585
900	884.681	1331.471	871.054	414.375	484.835	1207.191	-70.062
1000	921.822	1426.663	921.906	504.757	484.491	1287.481	-67.250
1100	952.878	1516.022	971.897	598.537	485.100	1367.769	-64.949
1200	979.065	1600.087	1020.778	695.171	486.501	1447.944	-63.026
1300	1001.303	1679.356	1068.419	794.219	488.490	1527.991	-61.394
1400	1020.304	1754.274	1114.757	895.324	490.919	1607.871	-59.989
1500	1036.630	1825.239	1159.778	998.191	493.694	1687.567	-58.765
1600	1050.733	1892.602	1203.493	1102.576	496.670	1767.060	-57.687
1700	1062.975	1956.679	1245.928	1208.275	499.764	1846.336	-56.730
1800	1073.653	2017.746	1287.124	1315.119	502.891	1925.500	-55.875
1900	1083.009	2076.051	1327.124	1422.962	506.016	2004.432	-55.105
2000	1091.243	2131.816	1365.975	1531.683	509.078	2083.229	-54.407
2100	1098.519	2185.238	1403.724	1641.179	511.989	2161.861	-53.772
2200	1104.976	2236.493	1440.420	1751.360	514.749	2240.361	-53.192
2300	1110.726	2285.740	1476.110	1862.150	517.351	2318.738	-52.659
2400	1115.866	2333.123	1510.838	1973.484	519.716	2396.953	-52.167
2500	1120.476	2378.770	1544.648	2085.306	521.857	2475.200	-51.715
2600	1124.625	2422.798	1577.581	2197.564	523.734	2553.237	-51.294
2700	1128.370	2465.313	1609.677	2310.217	525.351	2631.286	-50.904
2800	1131.762	2506.412	1640.973	2423.227	526.679	2709.305	-50.542
2900	1134.841	2546.181	1671.506	2536.559	527.686	2787.223	-50.202
3000	1137.645	2584.702	1701.307	2650.186	528.419	2865.140	-49.885
3100	1140.204	2622.048	1730.409	2764.080	528.793	2942.954	-49.587
3200	1142.545	2658.285	1758.842	2878.219	528.855	3020.842	-49.309
3300	1144.693	2693.476	1786.633	2992.583	528.582	3098.776	-49.049
3400	1146.667	2727.679	1813.810	3107.152	527.945	3176.628	-48.802
3500	1148.486	2760.944	1840.398	3221.911	526.949	3254.484	-48.570
3600	1150.165	2793.322	1866.421	3336.845	525.618	3332.470	-48.352
3700	1151.718	2824.857	1891.900	3451.940	523.917	3410.517	-48.147
3800	1153.156	2855.590	1916.858	3567.184	521.817	3488.547	-47.952
3900	1154.492	2885.562	1941.314	3682.567	519.363	3566.582	-47.768
4000	1155.733	2914.807	1965.287	3798.079	516.537	3644.838	-47.596
4100	1156.890	2943.359	1988.795	3913.711	513.300	3723.087	-47.432
4200	1157.968	2971.250	2011.856	4029.455	509.682	3801.409	-47.276
4300	1158.976	2998.510	2034.486	4145.303	505.668	3879.723	-47.128
4400	1159.919	3025.165	2056.700	4261.248	501.268	3958.237	-46.989
4500	1160.802	3051.242	2078.512	4377.284	496.498	4036.918	-46.858
4600	1161.630	3076.764	2099.937	4493.406	491.300	4115.717	-46.734
4700	1162.408	3101.755	2120.987	4609.609	485.690	4194.508	-46.616
4800	1163.140	3126.235	2141.676	4725.887	479.721	4273.539	-46.505
4900	1163.829	3150.226	2162.014	4842.235	473.310	4352.549	-46.398
5000	1164.479	3173.745	2182.014	4958.651	466.560	4431.902	-46.299

3.462. Naphtho[2,3-*a*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-58-5
Point Group: C₁

Length: 17.15 Å
Width: 11.34 Å
Breadth: 4.988 Å
L/B Ratio: 1.513

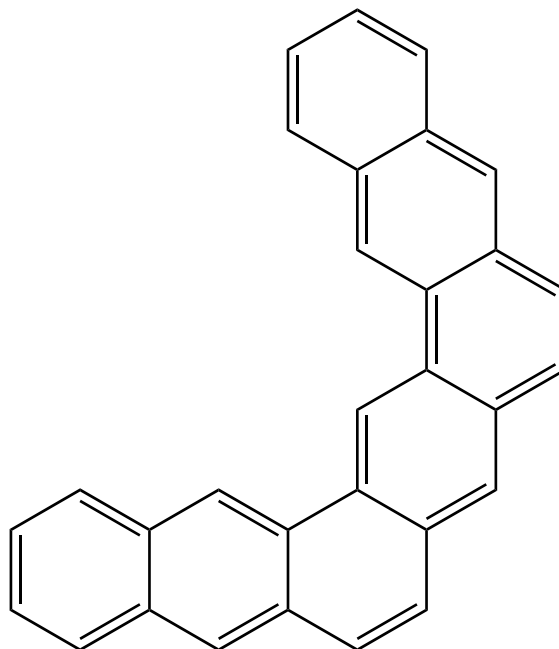
Cartesian coordinates:

C	-4.9373	3.5001	-0.5385	C	0.1771	-0.7611	0.1310	H	-7.0243	0.9520	0.3871
C	-6.1329	2.8181	-0.1829	C	1.3129	-1.5537	-0.1279	H	-2.8212	3.3562	-0.8520
C	-6.1083	1.4885	0.1155	C	1.6411	1.1437	0.5470	H	-5.7495	-1.1568	0.5507
C	-3.7470	2.8372	-0.5789	C	0.3967	0.5950	0.5221	H	-1.5598	1.3070	-0.5527
C	-3.6845	1.4450	-0.2612	C	2.7861	0.3846	0.1744	H	-4.5590	-3.2349	0.6339
C	-4.8773	0.7647	0.0770	C	2.6252	-0.9632	-0.1522	H	-2.4669	-4.5223	0.2600
C	-4.8210	-0.6128	0.3361	C	3.7787	-1.7364	-0.5037	H	-0.1691	-4.6281	-0.2743
C	-2.4647	0.7484	-0.2722	C	5.0170	-1.1810	-0.5358	H	2.0547	-3.5566	-0.5470
C	-2.3860	-0.6016	0.0524	C	4.0962	0.9843	0.1486	H	1.7947	2.1885	0.8590
C	-3.6112	-1.2950	0.2949	C	5.2065	0.1992	-0.2101	H	-0.4609	1.2072	0.8334
C	-3.6099	-2.7292	0.4221	C	6.4949	0.7824	-0.2429	H	3.6348	-2.7993	-0.7498
C	-2.4706	-3.4262	0.2333	C	6.6637	2.1081	0.0748	H	5.8941	-1.7782	-0.8102
C	-1.1346	-1.3524	0.0730	C	5.5549	2.8963	0.4372	H	7.3531	0.1618	-0.5247
C	-1.2180	-2.7479	0.0294	C	4.2970	2.3466	0.4741	H	7.6597	2.5620	0.0497
C	-0.0602	-3.5402	-0.1938	H	-4.9910	4.5670	-0.7786	H	5.7052	3.9511	0.6896
C	1.1616	-2.9536	-0.3240	H	-7.0722	3.3802	-0.1558	H	3.4213	2.9500	0.7583

Table 3.462: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*a*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.950	513.671	513.671	∞
100	125.207	375.939	868.381	-49.244	543.369	599.285	-313.028
200	246.322	497.820	652.666	-30.969	527.618	661.487	-172.759
250	316.708	560.291	627.914	-16.906	520.237	695.809	-145.378
298.15	385.343	621.956	621.956	0.000	513.671	730.236	-127.932
300	387.949	624.348	621.964	0.715	513.429	731.579	-127.377
350	456.479	689.349	626.941	21.843	507.386	768.429	-114.679
400	520.062	754.517	638.817	46.280	502.150	806.077	-105.261
450	577.691	819.159	655.271	73.749	497.631	844.344	-98.007
500	629.232	882.745	674.850	103.947	493.730	883.105	-92.255
600	715.738	1005.425	719.814	171.367	487.449	961.604	-83.713
700	784.247	1121.101	768.964	246.496	482.946	1041.016	-77.680
800	839.281	1229.544	819.834	327.769	480.012	1120.946	-73.189
900	884.205	1331.077	871.059	414.016	478.443	1201.154	-69.712
1000	921.375	1426.221	921.869	504.352	478.053	1281.486	-66.937
1100	952.459	1515.538	971.821	598.089	478.619	1361.819	-64.666
1200	978.674	1599.569	1020.667	694.682	479.980	1442.045	-62.769
1300	1000.938	1678.807	1068.275	793.692	481.931	1522.145	-61.159
1400	1019.963	1753.699	1114.584	894.761	484.325	1602.082	-59.773
1500	1036.313	1824.641	1159.577	997.595	487.067	1681.836	-58.566
1600	1050.437	1891.985	1203.266	1101.950	490.012	1761.390	-57.502
1700	1062.699	1956.044	1245.678	1207.621	493.077	1840.729	-56.558
1800	1073.396	2017.095	1286.852	1314.438	496.178	1919.957	-55.715
1900	1082.770	2075.388	1326.832	1422.256	499.278	1998.955	-54.954
2000	1091.020	2131.141	1365.664	1530.954	502.316	2077.819	-54.266
2100	1098.312	2184.552	1403.395	1640.428	505.206	2156.519	-53.639
2200	1104.781	2235.797	1440.075	1750.589	507.946	2235.088	-53.067
2300	1110.544	2285.037	1475.749	1861.361	510.529	2313.535	-52.541
2400	1115.696	2332.412	1510.463	1972.678	512.877	2391.821	-52.056
2500	1120.316	2378.052	1544.259	2084.482	515.001	2470.139	-51.610
2600	1124.475	2422.074	1577.180	2196.726	516.863	2548.248	-51.194
2700	1128.229	2464.584	1609.264	2309.364	518.465	2626.369	-50.809
2800	1131.629	2505.677	1640.549	2422.360	519.780	2704.462	-50.451
2900	1134.716	2545.442	1671.070	2535.679	520.773	2782.454	-50.116
3000	1137.526	2583.959	1700.861	2649.294	521.495	2860.445	-49.804
3100	1140.092	2621.301	1729.953	2763.176	521.857	2938.333	-49.510
3200	1142.439	2657.535	1758.377	2877.305	521.908	3016.296	-49.235
3300	1144.593	2692.723	1786.160	2991.658	521.625	3094.305	-48.978
3400	1146.572	2726.922	1813.329	3106.217	520.979	3172.233	-48.734
3500	1148.396	2760.185	1839.909	3220.967	519.973	3250.165	-48.505
3600	1150.079	2792.560	1865.924	3335.892	518.633	3328.226	-48.290
3700	1151.636	2824.093	1891.396	3450.979	516.924	3406.350	-48.088
3800	1153.078	2854.824	1916.347	3566.215	514.815	3484.457	-47.896
3900	1154.417	2884.794	1940.796	3681.591	512.354	3562.569	-47.714
4000	1155.662	2914.037	1964.763	3797.095	509.521	3640.901	-47.544
4100	1156.822	2942.588	1988.266	3912.720	506.276	3719.227	-47.383
4200	1157.903	2970.477	2011.321	4028.457	502.652	3797.627	-47.229
4300	1158.914	2997.735	2033.945	4144.299	498.632	3876.018	-47.083
4400	1159.859	3024.389	2056.153	4260.238	494.226	3954.610	-46.946
4500	1160.744	3050.464	2077.960	4376.268	489.449	4033.368	-46.817
4600	1161.575	3075.986	2099.380	4492.385	484.246	4112.245	-46.695
4700	1162.355	3100.975	2120.426	4608.582	478.631	4191.113	-46.578
4800	1163.089	3125.454	2141.110	4724.854	472.656	4270.222	-46.469
4900	1163.780	3149.444	2161.444	4841.198	466.240	4349.311	-46.363
5000	1164.431	3172.962	2181.440	4957.609	459.486	4428.742	-46.266

3.463. Naphtho[2,3-*a*]pentaphene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-73-4
Point Group: C_{2v}

Length: 16.79 Å
Width: 11.57 Å
Breadth: 3.885 Å
L/B Ratio: 1.451

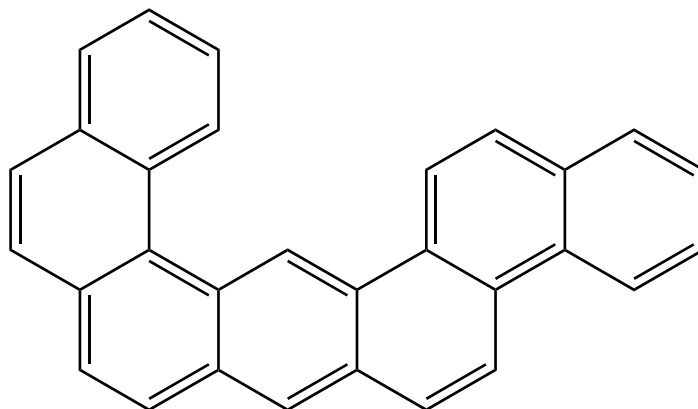
Cartesian coordinates:

C	5.0359	-3.5946	0.0000	C	-1.2175	1.2418	0.0000	H	7.1436	-0.9014	0.0000
C	6.2440	-2.8488	0.0000	C	-1.2162	2.6545	0.0000	H	2.8919	-3.5255	0.0000
C	6.2159	-1.4848	0.0000	C	-2.4708	3.3709	0.0000	H	5.8516	1.1904	0.0000
C	3.8292	-2.9579	0.0000	C	-3.6479	2.7139	0.0000	H	1.5914	-1.4257	0.0000
C	3.7664	-1.5325	0.0000	C	-2.4847	0.5256	0.0000	H	4.5917	3.2691	0.0000
C	4.9699	-0.7893	0.0000	C	-3.6999	1.2690	0.0000	H	2.4244	4.4719	0.0000
C	4.9155	0.6180	0.0000	C	-4.9170	0.6071	0.0000	H	-0.0050	4.4440	0.0000
C	2.5332	-0.8534	0.0000	C	-2.5313	-0.8589	0.0000	H	0.0004	-0.5484	0.0000
C	2.4834	0.5311	0.0000	C	-3.7629	-1.5408	0.0000	H	-2.4344	4.4665	0.0000
C	3.6970	1.2772	0.0000	C	-4.9681	-0.8004	0.0000	H	-4.5991	3.2589	0.0000
C	3.6417	2.7219	0.0000	C	-6.2125	-1.4988	0.0000	H	-5.8543	1.1773	0.0000
C	2.4632	3.3763	0.0000	C	-6.2375	-2.8629	0.0000	H	-1.5881	-1.4290	0.0000
C	1.2146	1.2444	0.0000	C	-5.0276	-3.6058	0.0000	H	-7.1416	-0.9175	0.0000
C	1.2102	2.6571	0.0000	C	-3.8224	-2.9664	0.0000	H	-7.1894	-3.4038	0.0000
C	-0.0038	3.3467	0.0000	H	5.0902	-4.6881	0.0000	H	-5.0794	-4.6995	0.0000
C	-0.0007	0.5587	0.0000	H	7.1972	-3.3876	0.0000	H	-2.8838	-3.5318	0.0000

Table 3.463: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*a*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.049	492.622	492.622	∞
100	125.501	371.723	864.871	-49.315	522.249	578.587	-302.217
200	246.734	493.890	648.880	-30.998	506.540	641.195	-167.460
250	317.005	556.442	624.108	-16.917	499.177	675.712	-141.179
298.15	385.485	618.147	618.147	0.000	492.622	710.323	-124.443
300	388.084	620.539	618.154	0.716	492.380	711.672	-123.911
350	456.436	685.548	623.132	21.846	486.339	748.712	-111.737
400	519.860	750.699	635.008	46.276	481.097	786.551	-102.711
450	577.369	815.310	651.460	73.732	476.564	825.010	-95.763
500	628.834	878.857	671.033	103.912	472.646	863.964	-90.256
600	715.299	1001.460	715.979	171.289	466.322	942.855	-82.081
700	783.860	1117.071	765.106	246.376	461.777	1022.667	-76.311
800	838.983	1225.468	815.951	327.614	458.808	1103.003	-72.017
900	884.000	1326.972	867.153	413.837	457.214	1183.620	-68.694
1000	921.253	1422.098	917.942	504.156	456.808	1264.364	-66.042
1100	952.404	1511.407	967.876	597.884	457.365	1345.110	-63.873
1200	978.670	1595.435	1016.706	694.474	458.723	1425.749	-62.060
1300	1000.973	1674.675	1064.301	793.486	460.676	1506.262	-60.521
1400	1020.025	1749.570	1110.598	894.561	463.075	1586.612	-59.196
1500	1036.394	1820.517	1155.582	997.402	465.824	1666.779	-58.041
1600	1050.531	1887.867	1199.263	1101.765	468.778	1746.745	-57.024
1700	1062.801	1951.932	1241.669	1207.446	471.853	1826.495	-56.120
1800	1073.502	2012.989	1282.838	1314.273	474.964	1906.134	-55.313
1900	1082.878	2071.287	1322.812	1422.102	478.075	1985.542	-54.585
2000	1091.128	2127.046	1361.640	1530.811	481.124	2064.816	-53.926
2100	1098.418	2180.462	1399.369	1640.296	484.025	2143.925	-53.326
2200	1104.885	2231.713	1436.046	1750.468	486.775	2222.904	-52.777
2300	1110.645	2280.956	1471.717	1861.250	489.368	2301.758	-52.273
2400	1115.793	2328.336	1506.429	1972.576	491.726	2380.452	-51.808
2500	1120.411	2373.980	1540.224	2084.391	493.860	2459.178	-51.381
2600	1124.566	2418.006	1573.143	2196.643	495.731	2537.694	-50.982
2700	1128.317	2460.519	1605.226	2309.290	497.342	2616.222	-50.613
2800	1131.713	2501.615	1636.510	2422.295	498.665	2694.721	-50.270
2900	1134.796	2541.383	1667.031	2535.622	499.667	2773.119	-49.948
3000	1137.603	2579.903	1696.821	2649.245	500.396	2851.515	-49.648
3100	1140.166	2617.247	1725.913	2763.135	500.767	2929.809	-49.366
3200	1142.510	2653.483	1754.336	2877.270	500.824	3008.177	-49.102
3300	1144.661	2688.674	1782.119	2991.631	500.548	3086.592	-48.856
3400	1146.637	2722.875	1809.288	3106.197	499.909	3164.924	-48.622
3500	1148.458	2756.140	1835.867	3220.953	498.910	3243.261	-48.402
3600	1150.139	2788.517	1861.882	3335.884	497.575	3321.727	-48.196
3700	1151.693	2820.051	1887.354	3450.976	495.872	3400.255	-48.002
3800	1153.133	2850.784	1912.305	3566.218	493.769	3478.766	-47.818
3900	1154.470	2880.754	1936.754	3681.599	491.313	3557.281	-47.643
4000	1155.713	2909.999	1960.722	3797.109	488.485	3636.018	-47.481
4100	1156.870	2938.551	1984.224	3912.739	485.246	3714.747	-47.325
4200	1157.950	2966.442	2007.280	4028.481	481.627	3793.551	-47.179
4300	1158.959	2993.701	2029.904	4144.327	477.611	3872.346	-47.039
4400	1159.902	3020.356	2052.112	4260.270	473.209	3951.341	-46.907
4500	1160.786	3046.432	2073.920	4376.305	468.437	4030.503	-46.784
4600	1161.615	3071.954	2095.340	4492.426	463.238	4109.782	-46.667
4700	1162.394	3096.944	2116.385	4608.627	457.626	4189.054	-46.555
4800	1163.127	3121.424	2137.070	4724.903	451.656	4268.566	-46.451
4900	1163.816	3145.414	2157.404	4841.250	445.243	4348.057	-46.350
5000	1164.466	3168.933	2177.400	4957.665	438.493	4427.892	-46.257

3.464. Phenanthro[3,4-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-84-7
Point Group: C₁

Length: 16.81 Å
Width: 11.17 Å
Breadth: 5.060 Å
L/B Ratio: 1.505

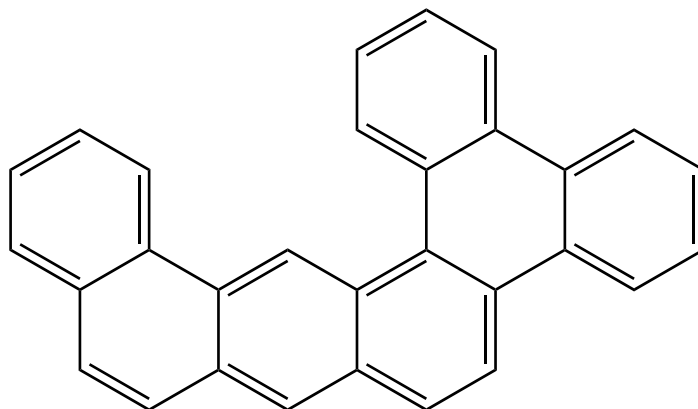
Cartesian coordinates:

C	6.7375	-1.6318	-0.2227	C	-1.6993	0.9971	0.0408	H	5.7476	1.6067	0.2447
C	6.8270	-0.2410	-0.0113	C	-1.5812	2.4114	0.1423	H	5.4310	-3.3146	-0.5029
C	5.6895	0.5200	0.0798	C	-2.7517	3.2383	0.0506	H	0.9160	-1.8117	-0.3650
C	5.5103	-2.2340	-0.3384	C	-3.9555	2.6813	-0.2077	H	2.9949	-3.1658	-0.5286
C	4.3241	-1.4647	-0.2469	C	-3.0261	0.4023	-0.0259	H	4.2550	2.5784	0.3645
C	4.4087	-0.0755	-0.0363	C	-4.1050	1.2547	-0.2740	H	2.1801	3.9461	0.5126
C	1.9072	-1.3404	-0.2765	C	-5.3974	0.7377	-0.5898	H	-0.2571	4.1030	0.3701
C	3.0428	-2.0831	-0.3652	C	-5.6196	-0.6013	-0.6066	H	-0.5557	-0.8287	-0.2448
C	1.9624	0.0708	-0.0660	C	-3.3088	-1.0055	0.1451	H	-2.6369	4.3232	0.1559
C	3.2003	0.6998	0.0546	C	-4.5868	-1.4983	-0.1999	H	-4.8471	3.3042	-0.3459
C	3.2594	2.1180	0.2697	C	-4.8767	-2.8813	-0.0955	H	-6.2001	1.4431	-0.8352
C	2.1320	2.8631	0.3508	C	-3.9454	-3.7525	0.4073	H	-6.5950	-1.0107	-0.8932
C	0.7461	0.8511	0.0274	C	-2.7013	-3.2603	0.8434	H	-5.8631	-3.2411	-0.4107
C	0.8401	2.2496	0.2240	C	-2.3957	-1.9285	0.7164	H	-4.1643	-4.8218	0.4897
C	-0.3274	3.0131	0.2628	H	7.6559	-2.2235	-0.2931	H	-1.9798	-3.9504	1.2935
C	-0.5172	0.2604	-0.0671	H	7.8137	0.2248	0.0791	H	-1.4245	-1.5724	1.0866

Table 3.464: Table of thermodynamic data as a function of temperature for Phenanthro[3,4-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.058	508.125	508.125	∞
100	125.641	377.370	870.240	-49.287	537.780	593.553	-310.034
200	246.503	499.436	654.370	-30.987	522.054	655.600	-171.222
250	316.882	561.946	629.604	-16.915	514.682	689.840	-144.131
298.15	385.532	623.643	623.643	0.000	508.125	724.187	-126.872
300	388.138	626.036	623.651	0.716	507.883	725.526	-126.323
350	456.693	691.068	628.630	21.853	501.850	762.291	-113.763
400	520.297	756.266	640.512	46.302	496.625	799.852	-104.448
450	577.941	820.937	656.974	73.783	492.118	838.032	-97.274
500	629.487	884.549	676.561	103.994	488.231	876.702	-91.587
600	715.986	1007.276	721.545	171.439	481.974	955.019	-83.140
700	784.473	1122.989	770.715	246.591	477.495	1034.244	-77.175
800	839.481	1231.460	821.603	327.885	474.582	1113.984	-72.734
900	884.380	1333.015	872.847	414.152	473.032	1193.999	-69.296
1000	921.527	1428.176	923.673	504.504	472.658	1274.136	-66.553
1100	952.591	1517.507	973.639	598.255	473.238	1354.273	-64.308
1200	978.789	1601.548	1022.498	694.860	474.612	1434.302	-62.432
1300	1001.038	1680.795	1070.118	793.881	476.574	1514.203	-60.840
1400	1020.052	1755.694	1116.437	894.960	478.977	1593.941	-59.469
1500	1036.391	1826.642	1161.440	997.802	481.727	1673.496	-58.275
1600	1050.506	1893.990	1205.138	1102.164	484.680	1752.849	-57.223
1700	1062.762	1958.053	1247.558	1207.842	487.751	1831.987	-56.289
1800	1073.452	2019.108	1288.739	1314.664	490.858	1911.014	-55.455
1900	1082.820	2077.403	1328.725	1422.488	493.964	1989.810	-54.703
2000	1091.066	2133.159	1367.563	1531.191	497.007	2068.473	-54.022
2100	1098.353	2186.572	1405.301	1640.669	499.901	2146.971	-53.402
2200	1104.819	2237.820	1441.986	1750.834	502.645	2225.338	-52.835
2300	1110.579	2287.060	1477.665	1861.610	505.231	2303.582	-52.315
2400	1115.727	2334.437	1512.383	1972.930	507.582	2381.666	-51.835
2500	1120.346	2380.079	1546.183	2084.738	509.710	2459.781	-51.393
2600	1124.502	2424.102	1579.108	2196.984	511.574	2537.687	-50.982
2700	1128.255	2466.612	1611.196	2309.625	513.179	2615.606	-50.601
2800	1131.652	2507.707	1642.484	2422.623	514.496	2693.496	-50.247
2900	1134.738	2547.473	1673.009	2535.945	515.492	2771.285	-49.915
3000	1137.547	2585.990	1702.803	2649.561	516.216	2849.073	-49.606
3100	1140.111	2623.332	1731.898	2763.446	516.580	2926.758	-49.315
3200	1142.457	2659.567	1760.325	2877.576	516.633	3004.517	-49.043
3300	1144.610	2694.756	1788.110	2991.931	516.351	3082.323	-48.788
3400	1146.588	2728.956	1815.281	3106.492	515.707	3160.048	-48.547
3500	1148.411	2762.219	1841.864	3221.243	514.703	3237.777	-48.320
3600	1150.093	2794.595	1867.881	3336.170	513.364	3315.634	-48.108
3700	1151.649	2826.127	1893.355	3451.258	511.656	3393.555	-47.907
3800	1153.091	2856.859	1918.308	3566.496	509.549	3471.458	-47.718
3900	1154.429	2886.829	1942.759	3681.872	507.089	3549.366	-47.537
4000	1155.674	2916.072	1966.728	3797.378	504.257	3627.495	-47.369
4100	1156.833	2944.623	1990.232	3913.004	501.014	3705.617	-47.209
4200	1157.914	2972.513	2013.289	4028.742	497.391	3783.814	-47.058
4300	1158.924	2999.772	2035.915	4144.585	493.371	3862.001	-46.913
4400	1159.868	3026.426	2058.125	4260.525	488.966	3940.389	-46.777
4500	1160.754	3052.501	2079.933	4376.556	484.191	4018.944	-46.650
4600	1161.584	3078.023	2101.354	4492.674	478.988	4097.617	-46.529
4700	1162.364	3103.012	2122.401	4608.871	473.374	4176.282	-46.413
4800	1163.097	3127.492	2143.087	4725.145	467.401	4255.187	-46.305
4900	1163.788	3151.481	2163.422	4841.490	460.985	4334.072	-46.201
5000	1164.439	3174.999	2183.419	4957.901	454.232	4413.300	-46.104

3.465. Benzo[*g*]naphtho[2,1-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-57-4
Point Group: C₁

Length: 16.44 Å
Width: 10.86 Å
Breadth: 5.544 Å
L/B Ratio: 1.514

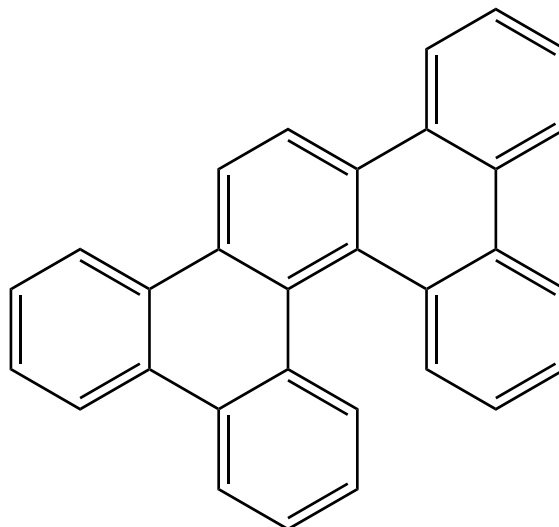
Cartesian coordinates:

C	5.9250	-2.0205	0.6967	C	-1.2139	0.3440	-0.2520	H	2.5175	-2.1603	0.5170
C	6.1106	-0.6770	0.4448	C	-2.2419	1.2736	-0.1250	H	4.4932	-3.6264	0.9246
C	3.5385	-1.7486	0.4995	C	-1.5703	-1.0603	-0.4046	H	6.2230	1.9506	-0.0701
C	4.6316	-2.5590	0.7238	C	-2.8784	-1.4865	-0.1000	H	4.2850	3.4521	-0.4624
C	3.7055	-0.3743	0.2429	C	-3.2133	-2.8520	-0.2001	H	1.8677	3.7946	-0.5642
C	5.0042	0.1627	0.2148	C	-2.3011	-3.7753	-0.6601	H	1.1251	-1.0699	0.2098
C	5.1964	1.5671	-0.0492	C	-1.0298	-3.3453	-1.0559	H	-0.5068	4.1949	-0.6017
C	4.1428	2.3837	-0.2631	C	-0.6783	-2.0182	-0.9312	H	-2.8178	3.3733	-0.2368
C	2.5664	0.4959	0.0049	C	-3.8970	-0.5177	0.2513	H	-4.2281	-3.1688	0.0857
C	2.7935	1.8752	-0.2346	C	-3.5997	0.8509	0.1631	H	-2.5687	-4.8341	-0.7343
C	1.7053	2.7198	-0.4129	C	-4.6246	1.7874	0.4132	H	-0.3168	-4.0663	-1.4692
C	1.2647	0.0067	0.0052	C	-5.8902	1.3756	0.7695	H	0.3228	-1.7061	-1.2599
C	0.1528	0.8301	-0.2331	C	-6.1758	0.0090	0.8875	H	-4.4003	2.8610	0.3257
C	0.3949	2.2202	-0.3832	C	-5.1939	-0.9218	0.6279	H	-6.6758	2.1127	0.9650
C	-0.7076	3.1290	-0.4451	H	6.7862	-2.6721	0.8765	H	-7.1800	-0.3131	1.1811
C	-1.9699	2.6722	-0.2630	H	7.1207	-0.2521	0.4221	H	-5.4118	-1.9979	0.7031

Table 3.465: Table of thermodynamic data as a function of temperature for Benzo[g]naphtho[2,1-b]chrysene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-57.138	512.405	512.405	∞
100	126.421	375.493	869.081	-49.359	541.988	597.949	-312.330
200	246.843	498.029	652.996	-30.993	526.328	660.156	-172.411
250	316.922	560.580	628.229	-16.912	518.965	694.465	-145.097
298.15	385.423	622.269	622.269	0.000	512.405	728.877	-127.694
300	388.026	624.661	622.277	0.715	512.164	730.219	-127.140
350	456.535	689.672	627.254	21.846	506.123	767.053	-114.474
400	520.148	754.849	639.132	46.287	500.891	804.685	-105.079
450	577.819	819.503	655.589	73.761	496.376	842.935	-97.843
500	629.395	883.104	675.171	103.967	492.484	881.678	-92.106
600	715.934	1005.819	720.144	171.405	486.221	960.139	-83.586
700	784.435	1121.524	769.306	246.553	481.737	1039.511	-77.568
800	839.440	1229.991	820.187	327.843	478.820	1119.397	-73.088
900	884.330	1331.541	871.424	414.105	477.266	1199.559	-69.619
1000	921.468	1426.696	922.245	504.451	476.886	1279.845	-66.851
1100	952.524	1516.021	972.206	598.196	477.460	1360.130	-64.586
1200	978.716	1600.056	1021.060	694.794	478.826	1440.308	-62.694
1300	1000.963	1679.297	1068.675	793.808	480.781	1520.359	-61.088
1400	1019.975	1754.190	1114.991	894.879	483.176	1600.246	-59.705
1500	1036.315	1825.132	1159.990	997.714	485.919	1679.952	-58.500
1600	1050.432	1892.476	1203.683	1102.068	488.864	1759.456	-57.439
1700	1062.689	1956.534	1246.100	1207.738	491.928	1838.746	-56.497
1800	1073.382	2017.585	1287.278	1314.554	495.028	1917.925	-55.656
1900	1082.753	2075.877	1327.261	1422.371	498.127	1996.874	-54.897
2000	1091.001	2131.629	1366.095	1531.067	501.163	2075.689	-54.210
2100	1098.292	2185.039	1403.830	1640.539	504.051	2154.340	-53.585
2200	1104.761	2236.284	1440.512	1750.698	506.789	2232.861	-53.014
2300	1110.523	2285.522	1476.188	1861.468	509.370	2311.259	-52.489
2400	1115.675	2332.896	1510.904	1972.782	511.715	2389.496	-52.005
2500	1120.296	2378.536	1544.702	2084.585	513.838	2467.766	-51.560
2600	1124.455	2422.557	1577.624	2196.826	515.697	2545.827	-51.145
2700	1128.210	2465.066	1609.709	2309.462	517.298	2623.900	-50.761
2800	1131.610	2506.159	1640.996	2422.456	518.610	2701.945	-50.404
2900	1134.697	2545.923	1671.518	2535.774	519.602	2779.888	-50.070
3000	1137.508	2584.439	1701.310	2649.386	520.321	2857.831	-49.758
3100	1140.074	2621.780	1730.404	2763.267	520.683	2935.672	-49.465
3200	1142.423	2658.014	1758.828	2877.394	520.731	3013.586	-49.191
3300	1144.576	2693.201	1786.612	2991.745	520.447	3091.548	-48.934
3400	1146.556	2727.400	1813.782	3106.303	519.799	3169.428	-48.691
3500	1148.380	2760.663	1840.362	3221.052	518.792	3247.312	-48.462
3600	1150.064	2793.038	1866.378	3335.975	517.450	3325.326	-48.248
3700	1151.622	2824.570	1891.851	3451.060	515.739	3403.402	-48.046
3800	1153.065	2855.301	1916.802	3566.295	513.630	3481.461	-47.855
3900	1154.404	2885.270	1941.252	3681.670	511.167	3559.525	-47.674
4000	1155.649	2914.513	1965.219	3797.173	508.332	3637.810	-47.504
4100	1156.809	2943.063	1988.722	3912.797	505.087	3716.088	-47.343
4200	1157.891	2970.952	2011.778	4028.532	501.461	3794.440	-47.190
4300	1158.902	2998.210	2034.403	4144.373	497.440	3872.784	-47.044
4400	1159.848	3024.864	2056.611	4260.311	493.033	3951.328	-46.907
4500	1160.734	3050.939	2078.419	4376.340	488.255	4030.039	-46.779
4600	1161.565	3076.460	2099.839	4492.456	483.051	4108.869	-46.657
4700	1162.346	3101.449	2120.885	4608.652	477.435	4187.690	-46.540
4800	1163.080	3125.928	2141.569	4724.923	471.459	4266.751	-46.431
4900	1163.771	3149.917	2161.904	4841.266	465.042	4345.792	-46.326
5000	1164.423	3173.435	2181.900	4957.676	458.287	4425.176	-46.229

3.466. Dibenzo[*f,j*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 188-67-0
Point Group: C₂

Length: 15.76 Å
Width: 10.24 Å
Breadth: 7.004 Å
L/B Ratio: 1.539

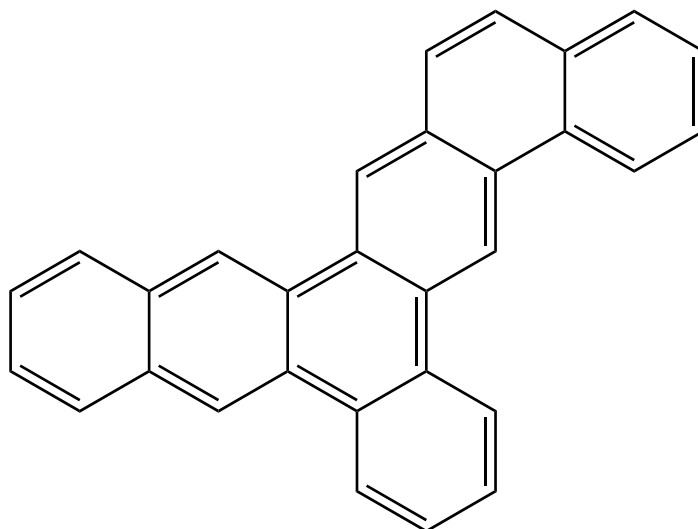
Cartesian coordinates:

C	3.6107	2.1138	0.7853	C	-3.5669	-0.2134	0.0693	H	-5.5046	0.7349	0.1964
C	2.8777	0.9799	0.3890	C	-2.8441	-1.4080	0.2121	H	-2.9626	-3.5247	0.6445
C	1.4768	0.9769	0.5154	C	-4.9524	-0.2104	0.3113	H	-4.7013	2.1132	-0.6345
C	0.8635	2.0624	1.1715	C	-5.6071	-1.3712	0.6701	H	-3.5582	4.0713	-1.6751
C	1.6004	3.1523	1.5898	C	-4.8929	-2.5691	0.7842	H	-1.1056	3.9871	-2.0963
C	2.9809	3.1935	1.3685	C	-3.5318	-2.5867	0.5561	H	-0.2185	2.0361	1.3555
C	0.7087	-0.1883	0.0926	C	-3.6108	2.1135	-0.7853	H	1.2389	-3.5599	-0.1729
C	1.3990	-1.4008	-0.0564	C	-2.9810	3.1933	-1.3683	H	-1.2385	-3.5600	0.1731
C	2.8441	-1.4077	-0.2122	C	-1.6006	3.1522	-1.5895	H	5.5046	0.7353	-0.1965
C	3.5668	-0.2131	-0.0695	C	-0.8636	2.0624	-1.1711	H	6.6851	-1.3592	-0.8612
C	-0.7087	-0.1883	-0.0925	C	4.9524	-0.2099	-0.3116	H	5.4171	-3.4901	-1.0582
C	-1.3989	-1.4009	0.0565	C	5.6071	-1.3707	-0.6705	H	2.9628	-3.5244	-0.6444
C	-0.6811	-2.6162	0.0737	C	4.8930	-2.5687	-0.7846	H	0.2185	2.0362	-1.3551
C	0.6814	-2.6162	-0.0735	C	3.5319	-2.5864	-0.5562	H	1.1054	3.9870	2.0969
C	-1.4769	0.9768	-0.5152	H	-5.4170	-3.4906	1.0577	H	3.5580	4.0716	1.6751
C	-2.8778	0.9797	-0.3891	H	-6.6850	-1.3598	0.8608	H	4.7012	2.1136	0.6342

Table 3.466: Table of thermodynamic data as a function of temperature for Dibenzof[*f,j*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.274	534.706	534.706	∞
100	127.639	366.341	861.440	-49.510	564.138	621.014	-324.378
200	247.545	489.627	644.825	-31.040	548.582	684.090	-178.662
250	317.360	552.303	620.026	-16.931	541.247	718.816	-150.185
298.15	385.775	614.060	614.060	0.000	534.706	753.625	-132.029
300	388.377	616.455	614.068	0.716	534.465	754.982	-131.451
350	456.909	681.520	619.050	21.865	528.442	792.225	-118.231
400	520.583	746.751	630.937	46.325	523.230	830.263	-108.419
450	578.313	811.460	647.408	73.823	518.739	868.917	-100.859
500	629.929	875.115	667.007	104.054	514.872	908.061	-94.862
600	716.479	997.929	712.018	171.547	508.663	987.316	-85.952
700	784.932	1113.716	761.219	246.748	504.232	1067.472	-79.654
800	839.864	1222.244	812.139	328.084	501.362	1148.136	-74.964
900	884.678	1323.839	863.412	414.384	499.846	1229.071	-71.332
1000	921.747	1419.028	914.265	504.762	499.498	1310.124	-68.432
1100	952.745	1508.376	964.256	598.532	500.096	1391.175	-66.060
1200	978.890	1592.428	1013.137	695.150	501.482	1472.116	-64.078
1300	1001.098	1671.682	1060.775	794.179	503.452	1552.929	-62.396
1400	1020.081	1746.584	1107.111	895.262	505.859	1633.578	-60.948
1500	1036.397	1817.533	1152.128	998.106	508.612	1714.044	-59.687
1600	1050.495	1884.881	1195.839	1102.468	511.564	1794.308	-58.577
1700	1062.738	1948.943	1238.270	1208.143	514.634	1874.357	-57.591
1800	1073.420	2009.996	1279.461	1314.963	517.738	1954.295	-56.711
1900	1082.782	2068.290	1319.456	1422.783	520.840	2034.003	-55.917
2000	1091.024	2124.043	1358.302	1531.482	523.879	2113.577	-55.200
2100	1098.308	2177.454	1396.046	1640.956	526.769	2192.986	-54.546
2200	1104.773	2228.700	1432.737	1751.117	529.508	2272.266	-53.949
2300	1110.532	2277.938	1468.422	1861.887	532.090	2351.422	-53.401
2400	1115.681	2325.313	1503.145	1973.203	534.436	2430.418	-52.896
2500	1120.300	2370.952	1536.950	2085.006	536.559	2509.446	-52.431
2600	1124.457	2414.974	1569.879	2197.247	538.419	2588.265	-51.998
2700	1128.210	2457.483	1601.970	2309.884	540.019	2667.097	-51.597
2800	1131.609	2498.575	1633.262	2422.878	541.332	2745.900	-51.224
2900	1134.696	2538.340	1663.790	2536.195	542.324	2824.601	-50.876
3000	1137.506	2576.856	1693.587	2649.807	543.043	2903.303	-50.550
3100	1140.072	2614.197	1722.685	2763.688	543.404	2981.901	-50.244
3200	1142.419	2650.430	1751.113	2877.814	543.452	3060.574	-49.958
3300	1144.573	2685.618	1778.901	2992.166	543.167	3139.294	-49.690
3400	1146.553	2719.817	1806.074	3106.723	542.519	3217.933	-49.436
3500	1148.376	2753.079	1832.659	3221.471	541.511	3296.575	-49.198
3600	1150.060	2785.454	1858.678	3336.394	540.169	3375.347	-48.974
3700	1151.617	2816.986	1884.154	3451.479	538.458	3454.182	-48.763
3800	1153.060	2847.717	1909.108	3566.714	536.348	3532.999	-48.563
3900	1154.400	2877.685	1933.561	3682.087	533.885	3611.822	-48.374
4000	1155.645	2906.928	1957.531	3797.590	531.050	3690.865	-48.197
4100	1156.805	2935.479	1981.036	3913.214	527.804	3769.901	-48.028
4200	1157.887	2963.368	2004.094	4028.949	524.178	3849.012	-47.868
4300	1158.898	2990.626	2026.721	4144.789	520.156	3928.115	-47.716
4400	1159.844	3017.279	2048.932	4260.726	515.749	4007.417	-47.573
4500	1160.730	3043.354	2070.742	4376.755	510.971	4086.887	-47.438
4600	1161.561	3068.875	2092.164	4492.870	505.766	4166.475	-47.311
4700	1162.342	3093.864	2113.212	4609.066	500.149	4246.054	-47.189
4800	1163.076	3118.343	2133.898	4725.337	494.174	4325.874	-47.074
4900	1163.767	3142.332	2154.234	4841.680	487.756	4405.674	-46.964
5000	1164.419	3165.850	2174.232	4958.089	481.001	4485.816	-46.862

3.467. Dibenzo[*c,h*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-39-2
Point Group: C_s

Length: 18.03 Å
Width: 11.66 Å
Breadth: 3.886 Å
L/B Ratio: 1.546

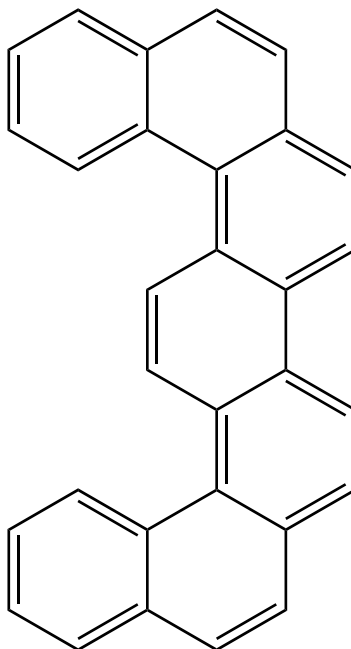
Cartesian coordinates:

C	5.8312	-2.8736	0.0000	C	0.1923	-0.3783	0.0000	H	6.4459	0.4898	0.0000
C	6.5541	-1.6541	0.0000	C	-0.4971	0.8598	0.0000	H	3.8984	-3.8077	0.0000
C	5.8950	-0.4574	0.0000	C	-1.8864	0.8652	0.0000	H	4.3264	1.7439	0.0000
C	4.4650	-2.8697	0.0000	C	-0.5364	-1.5621	0.0000	H	1.7807	-2.5498	0.0000
C	3.7515	-1.6369	0.0000	C	-1.9390	-1.5561	0.0000	H	3.4564	3.2948	0.0000
C	4.4710	-0.4231	0.0000	C	-2.6257	-0.3263	0.0000	H	2.2395	5.4617	0.0000
C	3.7621	0.7974	0.0000	C	-4.0345	-2.7815	0.0000	H	-0.2502	5.4911	0.0000
C	2.3405	-1.6006	0.0000	C	-2.6814	-2.7881	0.0000	H	-1.5175	3.3524	0.0000
C	1.6526	-0.4015	0.0000	C	-4.7670	-1.5437	0.0000	H	-2.4350	1.8268	0.0000
C	2.3800	0.8255	0.0000	C	-4.0734	-0.3209	0.0000	H	-0.0003	-2.5251	0.0000
C	0.2532	2.1114	0.0000	C	-4.8049	0.8847	0.0000	H	-4.6038	-3.7182	0.0000
C	1.6578	2.0944	0.0000	C	-6.1816	0.8677	0.0000	H	-2.1207	-3.7298	0.0000
C	2.3557	3.3125	0.0000	C	-6.8724	-0.3544	0.0000	H	-4.2472	1.8339	0.0000
C	1.6809	4.5202	0.0000	C	-6.1774	-1.5435	0.0000	H	-6.7449	1.8065	0.0000
C	0.2860	4.5367	0.0000	H	6.3857	-3.8178	0.0000	H	-7.9673	-0.3547	0.0000
C	-0.4167	3.3451	0.0000	H	7.6485	-1.6875	0.0000	H	-6.7126	-2.4999	0.0000

Table 3.467: Table of thermodynamic data as a function of temperature for Dibenzo[*c,h*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.402	488.103	488.103	∞
100	128.247	380.322	875.038	-49.472	517.574	573.052	-299.325
200	247.250	503.669	658.658	-30.998	502.022	634.721	-165.769
250	316.935	566.265	633.893	-16.907	494.668	668.747	-139.724
298.15	385.206	627.935	627.935	0.000	488.103	702.886	-123.140
300	387.803	630.326	627.943	0.715	487.861	704.217	-122.613
350	456.164	695.290	632.917	21.831	481.806	740.769	-110.551
400	519.689	760.411	644.786	46.250	476.552	778.122	-101.610
450	577.313	825.009	661.230	73.701	472.014	816.095	-94.728
500	628.874	888.556	680.795	103.880	468.095	854.564	-89.274
600	715.440	1011.176	725.732	171.267	461.781	932.485	-81.178
700	784.006	1126.811	774.855	246.369	457.251	1011.324	-75.464
800	839.087	1235.225	825.700	327.620	454.295	1090.685	-71.213
900	884.047	1336.737	876.904	413.850	452.709	1170.326	-67.923
1000	921.246	1431.866	927.694	504.171	452.305	1250.093	-65.297
1100	952.351	1521.172	977.630	597.896	452.859	1329.863	-63.149
1200	978.583	1605.193	1026.461	694.479	454.210	1409.526	-61.354
1300	1000.860	1684.425	1074.055	793.481	456.153	1489.063	-59.830
1400	1019.897	1759.312	1120.352	894.544	458.539	1568.438	-58.518
1500	1036.255	1830.249	1165.335	997.371	461.275	1647.632	-57.374
1600	1050.386	1897.590	1209.014	1101.720	464.215	1726.625	-56.367
1700	1062.655	1961.646	1251.418	1207.387	467.275	1805.404	-55.472
1800	1073.357	2022.695	1292.584	1314.199	470.372	1884.072	-54.673
1900	1082.735	2080.985	1332.557	1422.014	473.468	1962.509	-53.952
2000	1090.988	2136.737	1371.382	1530.709	476.503	2040.814	-53.299
2100	1098.283	2190.146	1409.108	1640.180	479.390	2118.954	-52.705
2200	1104.755	2241.391	1445.782	1750.338	482.127	2196.964	-52.161
2300	1110.520	2290.629	1481.451	1861.107	484.708	2274.852	-51.662
2400	1115.674	2338.003	1516.160	1972.422	487.053	2352.578	-51.201
2500	1120.297	2383.642	1549.952	2084.224	489.176	2430.338	-50.778
2600	1124.457	2427.664	1582.869	2196.466	491.035	2507.887	-50.383
2700	1128.212	2470.172	1614.949	2309.102	492.636	2585.450	-50.018
2800	1131.613	2511.265	1646.231	2422.096	493.949	2662.984	-49.678
2900	1134.701	2551.030	1676.749	2535.414	494.941	2740.417	-49.359
3000	1137.513	2589.546	1706.537	2649.027	495.661	2817.849	-49.062
3100	1140.079	2626.887	1735.627	2762.909	496.022	2895.179	-48.782
3200	1142.428	2663.121	1764.047	2877.036	496.071	2972.583	-48.521
3300	1144.582	2698.309	1791.828	2991.388	495.787	3050.034	-48.277
3400	1146.562	2732.508	1818.994	3105.946	495.140	3127.403	-48.046
3500	1148.386	2765.771	1845.572	3220.695	494.133	3204.776	-47.828
3600	1150.069	2798.146	1871.585	3335.619	492.792	3282.279	-47.624
3700	1151.627	2829.678	1897.055	3450.705	491.082	3359.845	-47.432
3800	1153.070	2860.409	1922.004	3565.940	488.973	3437.393	-47.249
3900	1154.409	2890.378	1946.451	3681.315	486.511	3514.946	-47.076
4000	1155.655	2919.621	1970.416	3796.819	483.676	3592.720	-46.915
4100	1156.814	2948.172	1993.917	3912.443	480.432	3670.487	-46.762
4200	1157.896	2976.061	2016.971	4028.179	476.807	3748.329	-46.616
4300	1158.907	3003.319	2039.593	4144.020	472.785	3826.162	-46.478
4400	1159.853	3029.973	2061.800	4259.959	468.379	3904.195	-46.348
4500	1160.739	3056.048	2083.606	4375.989	463.602	3982.395	-46.225
4600	1161.570	3081.569	2105.024	4492.105	458.398	4060.713	-46.110
4700	1162.350	3106.558	2126.069	4608.301	452.782	4139.024	-45.999
4800	1163.084	3131.038	2146.751	4724.573	446.807	4217.574	-45.896
4900	1163.775	3155.027	2167.085	4840.916	440.391	4296.104	-45.796
5000	1164.427	3178.545	2187.079	4957.327	433.636	4374.978	-45.704

3.468. Dibenzo[*a,o*]picene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-93-8
Point Group: C_2

Length: 16.39 Å
Width: 10.38 Å
Breadth: 4.739 Å
L/B Ratio: 1.579

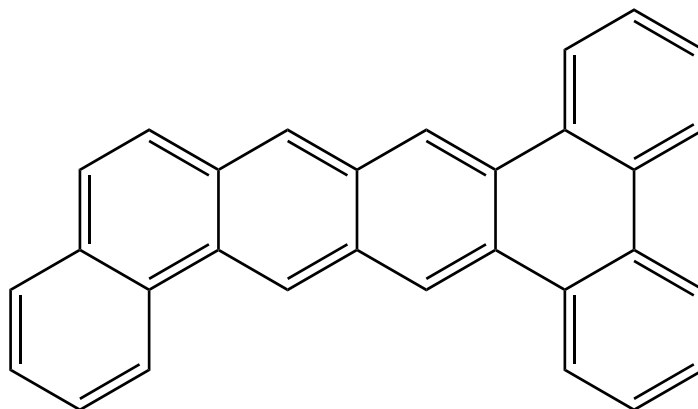
Cartesian coordinates:

C	5.3755	-3.0369	0.0804	C	-0.7212	1.6359	0.0924	H	2.1128	-2.1767	0.5002
C	3.9968	-3.1587	0.3208	C	-1.4361	0.4471	-0.1320	H	6.9947	-1.6759	-0.2918
C	3.1839	-2.0508	0.2923	C	-2.7937	2.8784	0.1951	H	5.4133	2.7603	-0.1171
C	5.9165	-1.7931	-0.1323	C	-1.4368	2.8529	0.2810	H	6.7916	0.7069	-0.3756
C	5.0943	-0.6422	-0.1331	C	-3.5302	1.6735	0.0197	H	0.8729	3.7795	0.4661
C	3.6959	-0.7594	0.0188	C	-2.8747	0.4355	-0.0340	H	3.3404	3.8246	0.2805
C	4.9529	1.7654	-0.1056	C	-5.7067	0.6467	-0.2344	H	1.2126	-1.5809	-0.9059
C	5.7066	0.6475	-0.2326	C	-4.9534	1.7649	-0.1076	H	-1.2136	-1.5805	-0.9064
C	3.5297	1.6734	0.0209	C	-5.0942	-0.6429	-0.1335	H	-3.3411	3.8246	0.2787
C	2.8743	0.4354	-0.0336	C	-3.6958	-0.7594	0.0192	H	-0.8736	3.7796	0.4654
C	1.4362	2.8528	0.2815	C	-3.1833	-2.0502	0.2947	H	-6.7916	0.7056	-0.3780
C	2.7931	2.8783	0.1964	C	-3.9957	-3.1584	0.3240	H	-5.4141	2.7596	-0.1198
C	0.7208	1.6357	0.0925	C	-5.5743	-3.0374	0.0824	H	-2.1123	-2.1746	0.5042
C	1.4357	0.4470	-0.1318	C	-5.9158	-1.7941	-0.1321	H	-3.5726	-4.1447	0.5417
C	0.6793	-0.6886	-0.5495	H	6.0082	-3.9301	0.0812	H	-6.0066	-3.9309	0.0839
C	-0.6798	-0.6886	-0.5496	H	3.5738	-4.1455	0.5367	H	-6.9939	-1.6775	-0.2923

Table 3.468: Table of thermodynamic data as a function of temperature for Dibenzo[*a,o*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.755	526.728	526.728	∞
100	124.474	366.564	858.182	-49.162	556.508	613.362	-320.381
200	245.917	488.065	642.764	-30.940	540.704	676.525	-176.687
250	316.404	550.455	618.033	-16.894	533.306	711.337	-148.623
298.15	385.176	612.078	612.078	0.000	526.728	746.239	-130.735
300	387.788	614.469	612.086	0.715	526.486	747.599	-130.166
350	456.482	679.457	617.061	21.839	520.439	784.944	-117.144
400	520.215	744.636	628.936	46.280	515.207	823.086	-107.482
450	577.962	809.303	645.392	73.760	510.698	861.847	-100.039
500	629.583	872.922	664.974	103.974	506.814	901.100	-94.135
600	716.155	995.674	709.953	171.432	500.572	980.577	-85.365
700	784.650	1111.414	759.124	246.603	496.110	1060.961	-79.168
800	839.633	1219.908	810.016	327.914	493.214	1141.857	-74.554
900	884.497	1321.479	861.264	414.193	491.677	1223.027	-70.981
1000	921.611	1416.650	912.095	504.555	491.314	1304.317	-68.129
1100	952.645	1505.988	962.066	598.313	491.900	1385.607	-65.796
1200	978.819	1590.032	1010.930	694.923	493.278	1466.787	-63.846
1300	1001.050	1669.281	1058.554	793.946	495.242	1547.840	-62.192
1400	1020.049	1744.180	1104.877	895.025	497.645	1628.729	-60.767
1500	1036.378	1815.127	1149.883	997.867	500.395	1709.435	-59.527
1600	1050.486	1882.475	1193.583	1102.227	503.346	1789.940	-58.434
1700	1062.736	1946.536	1236.006	1207.902	506.415	1870.230	-57.464
1800	1073.423	2007.590	1277.189	1314.722	509.519	1950.409	-56.598
1900	1082.789	2065.883	1317.177	1422.543	512.622	2030.357	-55.817
2000	1091.034	2121.637	1356.016	1531.243	515.662	2110.171	-55.111
2100	1098.320	2175.049	1393.755	1640.718	518.553	2189.821	-54.468
2200	1104.787	2226.295	1430.441	1750.879	521.294	2269.341	-53.880
2300	1110.546	2275.534	1466.120	1861.651	523.877	2348.738	-53.340
2400	1115.696	2322.909	1500.839	1972.968	526.224	2427.974	-52.842
2500	1120.315	2368.550	1534.640	2084.773	528.349	2507.243	-52.385
2600	1124.472	2412.572	1567.565	2197.016	530.210	2586.302	-51.958
2700	1128.225	2455.081	1599.654	2309.654	531.812	2665.373	-51.564
2800	1131.624	2496.174	1630.943	2422.649	533.126	2744.417	-51.197
2900	1134.710	2535.939	1661.467	2535.968	534.120	2823.358	-50.853
3000	1137.520	2574.456	1691.262	2649.582	534.840	2902.300	-50.532
3100	1140.086	2611.797	1720.357	2763.464	535.202	2981.138	-50.231
3200	1142.433	2648.031	1748.784	2877.592	535.252	3060.051	-49.949
3300	1144.586	2683.219	1776.569	2991.944	534.969	3139.011	-49.685
3400	1146.566	2717.418	1803.741	3106.503	534.322	3217.889	-49.436
3500	1148.389	2750.681	1830.323	3221.252	533.316	3296.772	-49.201
3600	1150.072	2783.056	1856.340	3336.176	531.975	3375.783	-48.980
3700	1151.629	2814.588	1881.815	3451.263	530.265	3454.858	-48.773
3800	1153.072	2845.320	1906.768	3566.498	528.156	3533.915	-48.576
3900	1154.411	2875.289	1931.219	3681.873	525.694	3612.977	-48.389
4000	1155.656	2904.532	1955.188	3797.377	522.860	3692.260	-48.215
4100	1156.815	2933.083	1978.692	3913.002	519.615	3771.536	-48.049
4200	1157.897	2960.972	2001.749	4028.738	515.990	3850.887	-47.892
4300	1158.908	2988.230	2024.374	4144.579	511.969	3930.228	-47.742
4400	1159.853	3014.884	2046.584	4260.517	507.563	4009.771	-47.601
4500	1160.739	3040.959	2068.393	4376.547	502.786	4089.480	-47.468
4600	1161.570	3066.480	2089.814	4492.663	497.581	4169.307	-47.343
4700	1162.350	3091.469	2110.861	4608.860	491.966	4249.126	-47.223
4800	1163.084	3115.948	2131.546	4725.132	485.991	4329.186	-47.110
4900	1163.775	3139.938	2151.881	4841.475	479.574	4409.225	-47.002
5000	1164.426	3163.456	2171.878	4957.885	472.820	4489.607	-46.902

3.469. Tribenzo[*a,c,j*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 215-96-3
Point Group: C_s

Length: 17.79 Å
Width: 11.38 Å
Breadth: 3.887 Å
L/B Ratio: 1.563

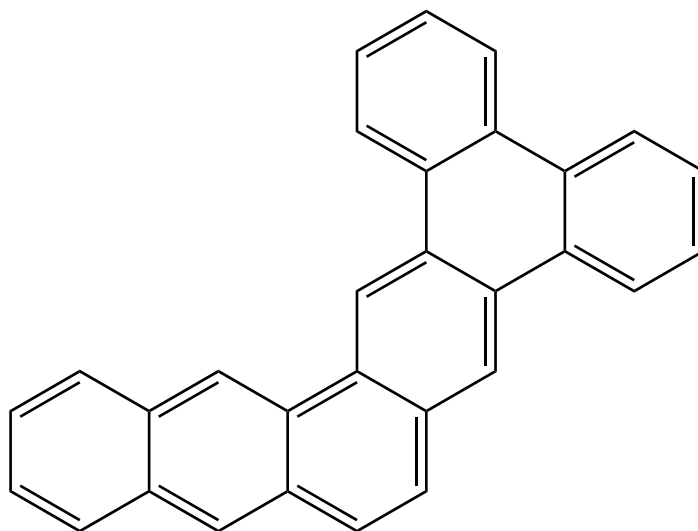
Cartesian coordinates:

C	7.1470	-1.3497	0.0000	C	-1.6666	-0.6195	0.0000	H	3.9259	-2.4843	0.0000
C	6.9074	0.0101	0.0000	C	-1.8786	0.7963	0.0000	H	6.2747	-3.3289	0.0000
C	4.7772	-1.7863	0.0000	C	-2.8163	-1.5188	0.0000	H	6.1978	2.5946	0.0000
C	6.0766	-2.2521	0.0000	C	-4.1222	-1.0010	0.0000	H	3.8815	3.4794	0.0000
C	4.5122	-0.4050	0.0000	C	-5.2104	-1.8882	0.0000	H	1.4790	3.1018	0.0000
C	5.5884	0.4983	0.0000	C	-5.0124	-3.2571	0.0000	H	2.2309	-1.8431	0.0000
C	5.3343	1.9193	0.0000	C	-3.7154	-3.7718	0.0000	H	-0.9540	2.7364	0.0000
C	4.0743	2.4002	0.0000	C	-2.6328	-2.9110	0.0000	H	-0.2139	-2.2035	0.0000
C	3.1482	0.1007	0.0000	C	-4.3382	0.4415	0.0000	H	-6.2315	-1.4773	0.0000
C	2.9344	1.5120	0.0000	C	-3.2414	1.3193	0.0000	H	-5.8707	-3.9366	0.0000
C	1.6464	2.0176	0.0000	C	-3.4738	2.7041	0.0000	H	-3.5565	-4.8549	0.0000
C	2.0606	-0.7544	0.0000	C	-4.7611	3.2099	0.0000	H	-1.6076	-3.3118	0.0000
C	0.7432	-0.2502	0.0000	C	-5.8504	2.3378	0.0000	H	-2.6110	3.3878	0.0000
C	0.5338	1.1495	0.0000	C	-5.6386	0.9710	0.0000	H	-4.9265	4.2921	0.0000
C	-0.7937	1.6461	0.0000	H	8.1745	-1.7279	0.0000	H	-6.8701	2.7360	0.0000
C	-0.3802	-1.1141	0.0000	H	7.7430	0.7193	0.0000	H	-6.4946	0.2789	0.0000

Table 3.469: Table of thermodynamic data as a function of temperature for Tribenzo[*a,c,j*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.804	496.182	496.182	∞
100	129.133	391.472	887.460	-49.599	525.525	579.888	-302.896
200	247.918	515.296	670.580	-31.057	510.041	640.416	-167.256
250	317.543	578.035	645.771	-16.934	502.720	673.856	-140.792
298.15	385.718	639.805	639.805	0.000	496.182	707.426	-123.935
300	388.310	642.199	639.812	0.716	495.941	708.735	-123.399
350	456.572	707.233	644.792	21.854	489.908	744.691	-111.137
400	520.014	772.403	656.673	46.292	484.673	781.445	-102.044
450	577.574	837.035	673.130	73.757	480.149	818.819	-95.044
500	629.084	900.607	692.710	103.948	476.242	856.686	-89.495
600	715.579	1023.259	737.672	171.352	469.945	933.400	-81.258
700	784.100	1138.911	786.817	246.466	465.427	1011.030	-75.442
800	839.149	1247.336	837.680	327.725	462.479	1089.180	-71.115
900	884.087	1348.854	888.899	413.960	460.898	1167.609	-67.765
1000	921.270	1443.986	939.702	504.284	460.496	1246.164	-65.092
1100	952.365	1533.294	989.647	598.011	461.052	1324.722	-62.904
1200	978.589	1617.316	1038.487	694.595	462.404	1403.173	-61.077
1300	1000.861	1696.548	1086.089	793.597	464.347	1481.498	-59.526
1400	1019.893	1771.435	1132.392	894.660	466.734	1559.661	-58.190
1500	1036.249	1842.372	1177.381	997.487	469.469	1637.642	-57.027
1600	1050.379	1909.712	1221.065	1101.835	472.408	1715.423	-56.002
1700	1062.646	1973.767	1263.473	1207.501	475.468	1792.989	-55.091
1800	1073.347	2034.816	1304.643	1314.312	478.563	1870.445	-54.278
1900	1082.725	2093.106	1344.618	1422.126	481.659	1947.671	-53.544
2000	1090.979	2148.857	1383.447	1530.820	484.693	2024.763	-52.880
2100	1098.273	2202.266	1421.175	1640.290	487.579	2101.692	-52.276
2200	1104.746	2253.510	1457.852	1750.447	490.315	2178.490	-51.723
2300	1110.511	2302.747	1493.523	1861.216	492.894	2255.165	-51.215
2400	1115.665	2350.121	1528.234	1972.529	495.239	2331.680	-50.747
2500	1120.288	2395.760	1562.028	2084.331	497.361	2408.227	-50.316
2600	1124.448	2439.781	1594.946	2196.571	499.219	2484.565	-49.915
2700	1128.204	2482.290	1627.028	2309.207	500.819	2560.916	-49.543
2800	1131.605	2523.383	1658.311	2422.200	502.131	2637.239	-49.197
2900	1134.693	2563.147	1688.830	2535.518	503.123	2713.460	-48.874
3000	1137.505	2601.663	1718.620	2649.130	503.842	2789.680	-48.572
3100	1140.072	2639.004	1747.710	2763.010	504.202	2865.798	-48.287
3200	1142.421	2675.237	1776.132	2877.137	504.251	2941.991	-48.022
3300	1144.575	2710.425	1803.913	2991.488	503.966	3018.230	-47.774
3400	1146.555	2744.624	1831.081	3106.046	503.318	3094.388	-47.538
3500	1148.380	2777.886	1857.659	3220.794	502.311	3170.549	-47.317
3600	1150.064	2810.261	1883.673	3335.717	500.969	3246.841	-47.109
3700	1151.621	2841.793	1909.144	3450.803	499.259	3323.194	-46.914
3800	1153.064	2872.524	1934.093	3566.038	497.149	3399.531	-46.729
3900	1154.404	2902.493	1958.541	3681.412	494.686	3475.873	-46.553
4000	1155.650	2931.736	1982.507	3796.915	491.851	3552.435	-46.389
4100	1156.810	2960.286	2006.009	3912.539	488.606	3628.991	-46.233
4200	1157.892	2988.176	2029.063	4028.275	484.981	3705.621	-46.085
4300	1158.903	3015.434	2051.686	4144.115	480.959	3782.243	-45.944
4400	1159.849	3042.087	2073.893	4260.053	476.552	3859.065	-45.812
4500	1160.735	3068.162	2095.699	4376.083	471.775	3936.053	-45.688
4600	1161.566	3093.683	2117.118	4492.198	466.570	4013.160	-45.570
4700	1162.346	3118.673	2138.163	4608.394	460.954	4090.259	-45.457
4800	1163.081	3143.152	2158.846	4724.666	454.979	4167.598	-45.352
4900	1163.772	3167.141	2179.180	4841.009	448.562	4244.917	-45.250
5000	1164.423	3190.659	2199.175	4957.419	441.807	4322.579	-45.157

3.470. Dibenzo[*a,c*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-37-0
Point Group: C_s

Length: 17.58 Å
Width: 11.15 Å
Breadth: 3.891 Å
L/B Ratio: 1.577

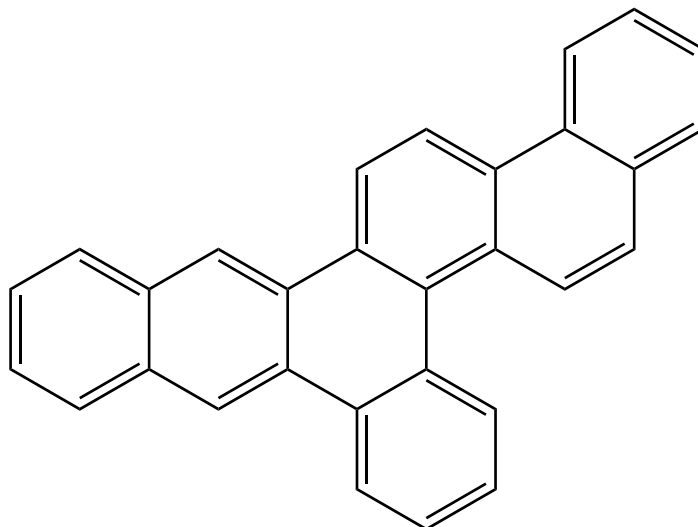
Cartesian coordinates:

C	6.3108	-2.1590	0.0000	C	-1.3843	-0.3316	0.0000	H	7.1200	1.1638	0.0000
C	7.1038	-0.9813	0.0000	C	-1.9687	0.9546	0.0000	H	4.3292	-2.9805	0.0000
C	6.5155	0.2497	0.0000	C	-2.2330	-1.5146	0.0000	H	5.0803	2.5364	0.0000
C	4.9490	-2.0769	0.0000	C	-3.6312	-1.3779	0.0000	H	2.2782	-1.6040	0.0000
C	4.3037	-0.8042	0.0000	C	-4.4323	-2.5333	0.0000	H	3.0748	3.9105	0.0000
C	5.0935	0.3694	0.0000	C	-3.8628	-3.7917	0.0000	H	0.6037	4.1117	0.0000
C	4.4637	1.6289	0.0000	C	-2.4719	-3.9276	0.0000	H	-1.6021	3.0812	0.0000
C	2.9004	-0.6944	0.0000	C	-1.6701	-2.8030	0.0000	H	0.4700	-1.4548	0.0000
C	2.2841	0.5465	0.0000	C	-4.2339	-0.0526	0.0000	H	-5.5271	-2.4188	0.0000
C	3.0816	1.7269	0.0000	C	-3.4184	1.0915	0.0000	H	-4.4981	-4.6833	0.0000
C	2.4353	3.0201	0.0000	C	-4.0205	2.3621	0.0000	H	-2.0212	-4.9253	0.0000
C	1.0915	3.1301	0.0000	C	-5.3952	2.4960	0.0000	H	-0.5736	-2.9018	0.0000
C	0.8345	0.6740	0.0000	C	-6.2063	1.3580	0.0000	H	-3.3752	3.2539	0.0000
C	0.2485	1.9572	0.0000	C	-5.6313	0.1021	0.0000	H	-5.8513	3.4913	0.0000
C	-1.1421	2.0797	0.0000	H	6.8114	-3.1328	0.0000	H	-7.2959	1.4646	0.0000
C	0.0062	-0.4495	0.0000	H	8.1943	-1.0789	0.0000	H	-6.2640	-0.7986	0.0000

Table 3.470: Table of thermodynamic data as a function of temperature for Dibenzo[*a,c*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.528	489.960	489.960	∞
100	128.357	387.095	881.597	-49.450	519.452	574.253	-299.953
200	247.190	510.449	665.329	-30.976	503.900	635.244	-165.905
250	316.715	573.015	640.584	-16.892	496.540	668.931	-139.763
298.15	384.805	634.632	634.632	0.000	489.960	702.746	-123.116
300	387.394	637.020	634.639	0.714	489.717	704.065	-122.586
350	455.595	701.908	639.608	21.805	483.637	740.284	-110.479
400	519.006	766.945	651.462	46.193	478.352	777.308	-101.504
450	576.563	831.458	667.885	73.608	473.778	814.957	-94.596
500	628.093	894.924	687.426	103.749	469.821	853.105	-89.121
600	714.665	1017.402	732.307	171.057	463.428	930.397	-80.997
700	783.280	1132.920	781.372	246.084	458.823	1008.620	-75.263
800	838.423	1241.241	832.159	327.266	455.798	1087.374	-70.997
900	883.446	1342.679	883.310	413.432	454.148	1166.417	-67.696
1000	920.703	1437.748	934.051	503.697	453.687	1245.593	-65.062
1100	951.861	1527.004	983.941	597.370	454.189	1324.777	-62.907
1200	978.140	1610.985	1032.730	693.906	455.494	1403.859	-61.107
1300	1000.459	1690.184	1080.286	792.866	457.394	1482.819	-59.579
1400	1019.533	1765.042	1126.549	893.890	459.742	1561.620	-58.264
1500	1035.924	1835.955	1171.500	996.683	462.443	1640.242	-57.117
1600	1050.084	1903.275	1215.150	1101.001	465.352	1718.665	-56.108
1700	1062.378	1967.314	1257.526	1206.638	468.383	1796.876	-55.210
1800	1073.103	2028.348	1298.668	1313.424	471.453	1874.978	-54.409
1900	1082.502	2086.625	1338.617	1421.215	474.526	1952.851	-53.687
2000	1090.773	2142.365	1377.421	1529.887	477.538	2030.592	-53.033
2100	1098.084	2195.764	1415.127	1639.337	480.404	2108.170	-52.437
2200	1104.571	2247.000	1451.783	1749.476	483.122	2185.619	-51.892
2300	1110.350	2296.230	1487.435	1860.228	485.685	2262.946	-51.392
2400	1115.515	2343.597	1522.128	1971.526	488.014	2340.113	-50.930
2500	1120.148	2389.230	1555.905	2083.313	490.121	2417.313	-50.506
2600	1124.318	2433.246	1588.807	2195.540	491.966	2494.304	-50.110
2700	1128.083	2475.750	1620.875	2308.163	493.553	2571.309	-49.744
2800	1131.492	2516.838	1652.144	2421.145	494.854	2648.286	-49.403
2900	1134.587	2556.599	1682.650	2534.451	495.834	2725.161	-49.084
3000	1137.405	2595.111	1712.427	2648.053	496.543	2802.037	-48.787
3100	1139.978	2632.449	1741.506	2761.924	496.894	2878.810	-48.507
3200	1142.332	2668.680	1769.917	2876.041	496.933	2955.658	-48.245
3300	1144.491	2703.865	1797.688	2990.384	496.640	3032.553	-48.000
3400	1146.476	2738.061	1824.845	3104.934	495.984	3109.367	-47.769
3500	1148.305	2771.321	1851.414	3219.674	494.969	3186.185	-47.550
3600	1149.993	2803.694	1877.419	3334.590	493.620	3263.133	-47.346
3700	1151.554	2835.224	1902.881	3449.668	491.902	3340.144	-47.153
3800	1153.000	2865.953	1927.823	3564.897	489.786	3417.137	-46.971
3900	1154.343	2895.921	1952.263	3680.265	487.317	3494.136	-46.798
4000	1155.591	2925.162	1976.221	3795.762	484.476	3571.356	-46.636
4100	1156.754	2953.711	1999.716	3911.380	481.225	3648.569	-46.482
4200	1157.839	2981.599	2022.763	4027.111	477.595	3725.857	-46.337
4300	1158.852	3008.856	2045.380	4142.946	473.568	3803.136	-46.198
4400	1159.800	3035.508	2067.581	4258.879	469.156	3880.616	-46.068
4500	1160.688	3061.582	2089.381	4374.904	464.374	3958.263	-45.945
4600	1161.521	3087.102	2110.795	4491.015	459.165	4036.028	-45.830
4700	1162.304	3112.091	2131.834	4607.206	453.544	4113.785	-45.719
4800	1163.039	3136.569	2152.512	4723.474	447.565	4191.782	-45.615
4900	1163.732	3160.557	2172.840	4839.813	441.144	4269.759	-45.515
5000	1164.385	3184.074	2192.830	4956.219	434.385	4348.079	-45.423

3.471. Dibenzo[*b,f*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-68-7
Point Group: C₁

Length: 17.92 Å
Width: 11.40 Å
Breadth: 5.074 Å
L/B Ratio: 1.573

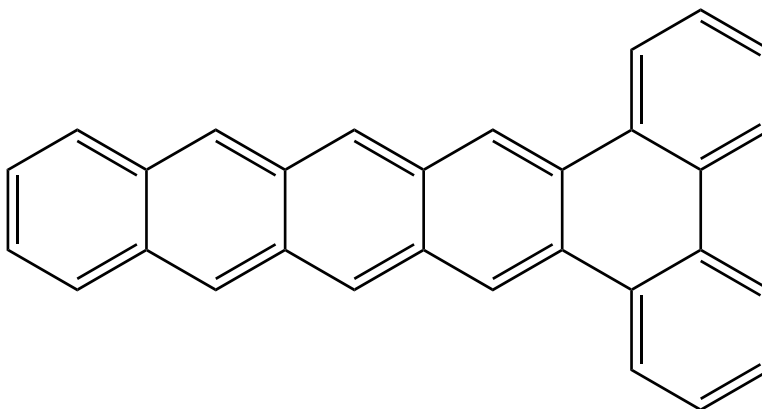
Cartesian coordinates:

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C	-6.6209	1.4609	0.4254	C	0.5561	-0.5601	-0.1238	H	-4.1746	3.7525	-0.2523
C	-5.8775	0.3164	0.4614	C	1.7424	1.9653	-0.5151	H	-4.1601	-1.7744	0.4280
C	-4.6588	2.7902	-0.0515	C	0.3819	1.8372	-0.5222	H	-1.9894	2.6421	-0.4089
C	-3.8561	1.6122	-0.0181	C	2.5575	0.8642	-0.1672	H	-3.2233	-3.2536	0.1035
C	-4.4705	0.3667	0.2373	C	1.9647	-0.3880	0.0793	H	-1.9128	-5.3354	-0.2754
C	-3.6789	-0.7988	0.2532	C	2.8052	-1.4270	0.6081	H	0.5318	-5.1826	-0.7337
C	-2.4628	1.6648	-0.2237	C	4.1385	-1.2592	0.7816	H	1.6736	-3.0084	-0.6680
C	-1.6859	0.5190	-0.1830	C	3.9872	1.0391	-0.0372	H	2.2218	2.9302	-0.7403
C	-2.3135	-0.7397	0.0343	C	4.7751	-0.0265	0.4281	H	-0.2549	2.7137	-0.7160
C	-0.1066	-1.8636	-0.1838	C	6.1729	0.1325	0.5540	H	2.3425	-2.3810	0.8963
C	-1.5054	-1.9484	-0.0430	C	6.7659	1.3280	0.2224	H	4.7555	-2.0627	1.2006
C	-2.1347	-3.2048	-0.0531	C	5.9821	2.3997	-0.2400	H	6.7750	-0.7075	0.9186
C	-1.4126	-4.3618	-0.2713	C	4.6200	2.2597	-0.3653	H	7.8494	1.4545	0.3164
C	-0.0412	-4.2765	-0.5110	H	-6.6266	3.6128	0.1408	H	6.4656	3.3471	-0.4998
C	0.5938	-3.0489	-0.4701	H	-7.7019	1.4297	0.5966	H	3.9992	3.0950	-0.7234

Table 3.471: Table of thermodynamic data as a function of temperature for Dibenzo[*b,f*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.264	515.917	515.917	∞
100	127.149	378.789	872.941	-49.415	545.444	601.075	-313.963
200	247.047	501.669	656.687	-31.003	529.829	662.929	-173.136
250	317.013	564.251	631.914	-16.916	522.473	697.055	-145.639
298.15	385.467	625.953	625.953	0.000	515.917	731.291	-128.116
300	388.069	628.345	625.960	0.716	515.675	732.625	-127.559
350	456.555	693.360	630.938	21.848	509.636	769.275	-114.806
400	520.156	758.539	642.817	46.289	504.405	806.723	-105.345
450	577.821	823.194	659.274	73.764	499.891	844.789	-98.058
500	629.395	886.795	678.857	103.969	495.998	883.347	-92.281
600	715.936	1009.509	723.831	171.407	489.735	961.439	-83.699
700	784.443	1125.216	772.993	246.556	485.252	1040.441	-77.637
800	839.455	1233.684	823.875	327.847	482.336	1119.959	-73.124
900	884.351	1335.236	875.113	414.111	480.784	1199.751	-69.630
1000	921.494	1430.394	925.934	504.460	480.407	1279.667	-66.842
1100	952.553	1519.721	975.896	598.207	480.983	1359.583	-64.560
1200	978.747	1603.759	1024.751	694.809	482.352	1439.390	-62.654
1300	1000.994	1683.002	1072.368	793.825	484.310	1519.071	-61.036
1400	1020.007	1757.898	1118.684	894.900	486.709	1598.587	-59.643
1500	1036.346	1828.842	1163.684	997.738	489.454	1677.922	-58.429
1600	1050.462	1896.188	1207.379	1102.095	492.403	1757.055	-57.361
1700	1062.718	1960.248	1249.796	1207.768	495.470	1835.974	-56.411
1800	1073.410	2021.301	1290.975	1314.587	498.572	1914.782	-55.564
1900	1082.780	2079.594	1330.959	1422.406	501.674	1993.359	-54.800
2000	1091.027	2135.347	1369.795	1531.105	504.713	2071.802	-54.109
2100	1098.316	2188.759	1407.530	1640.580	507.603	2150.081	-53.479
2200	1104.784	2240.005	1444.213	1750.741	510.344	2228.230	-52.904
2300	1110.545	2289.244	1479.890	1861.513	512.927	2306.256	-52.376
2400	1115.696	2336.619	1514.607	1972.830	515.274	2384.121	-51.888
2500	1120.316	2382.259	1548.405	2084.634	517.399	2462.019	-51.440
2600	1124.473	2426.281	1581.328	2196.877	519.260	2539.707	-51.022
2700	1128.227	2468.791	1613.415	2309.516	520.862	2617.408	-50.636
2800	1131.626	2509.884	1644.702	2422.511	522.177	2695.080	-50.276
2900	1134.713	2549.649	1675.225	2535.830	523.170	2772.651	-49.940
3000	1137.523	2588.166	1705.018	2649.444	523.891	2850.221	-49.626
3100	1140.089	2625.507	1734.112	2763.327	524.254	2927.689	-49.330
3200	1142.436	2661.741	1762.537	2877.455	524.304	3005.231	-49.054
3300	1144.589	2696.929	1790.321	2991.808	524.020	3082.819	-48.796
3400	1146.569	2731.129	1817.491	3106.367	523.374	3160.327	-48.552
3500	1148.392	2764.391	1844.072	3221.116	522.368	3237.838	-48.321
3600	1150.075	2796.767	1870.089	3336.041	521.027	3315.479	-48.105
3700	1151.632	2828.299	1895.562	3451.127	519.318	3393.182	-47.902
3800	1153.075	2859.030	1920.514	3566.363	517.209	3470.868	-47.709
3900	1154.414	2889.000	1944.964	3681.739	514.747	3548.559	-47.527
4000	1155.659	2918.243	1968.932	3797.243	511.914	3626.471	-47.356
4100	1156.818	2946.793	1992.435	3912.867	508.669	3704.376	-47.193
4200	1157.900	2974.683	2015.491	4028.604	505.045	3782.356	-47.040
4300	1158.911	3001.941	2038.116	4144.445	501.024	3860.326	-46.893
4400	1159.856	3028.595	2060.326	4260.384	496.618	3938.497	-46.755
4500	1160.742	3054.670	2082.133	4376.414	491.841	4016.836	-46.625
4600	1161.572	3080.191	2103.554	4492.530	486.637	4095.292	-46.503
4700	1162.353	3105.180	2124.600	4608.727	481.022	4173.740	-46.385
4800	1163.087	3129.660	2145.285	4724.999	475.047	4252.428	-46.275
4900	1163.778	3153.649	2165.620	4841.343	468.631	4331.096	-46.169
5000	1164.429	3177.167	2185.616	4957.754	461.876	4410.107	-46.071

3.472. Dibenzo[*a,c*]pentacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 216-08-0
Point Group: C_{2v}

Length: 18.35 Å
Width: 11.49 Å
Breadth: 3.890 Å
L/B Ratio: 1.597

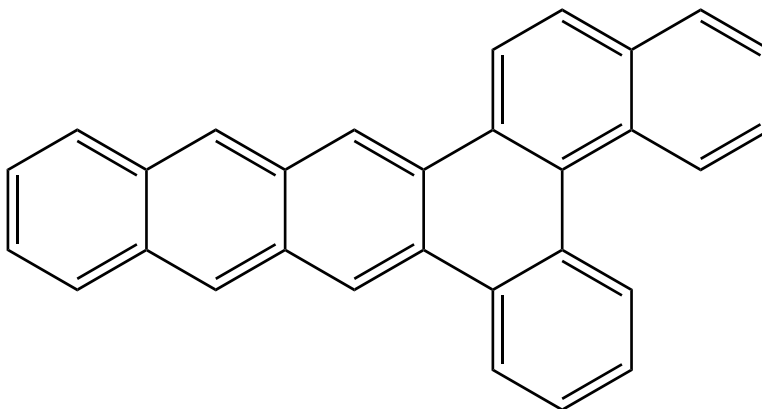
Cartesian coordinates:

C	-7.8043	0.7086	0.0000	C	1.9308	0.7228	0.0000	H	-6.6253	-2.5087	0.0000
C	-7.8030	-0.7230	0.0000	C	1.9322	-0.7194	0.0000	H	-6.6299	2.4964	0.0000
C	-6.6364	-1.4128	0.0000	C	3.2040	1.4399	0.0000	H	-4.1695	-2.5067	0.0000
C	-6.6390	1.4005	0.0000	C	4.4188	0.7341	0.0000	H	-4.1740	2.4989	0.0000
C	-5.3748	0.7110	0.0000	C	5.6255	1.4498	0.0000	H	-1.7182	-2.5045	0.0000
C	-5.3735	-0.7210	0.0000	C	5.6331	2.8339	0.0000	H	-1.7228	2.5012	0.0000
C	-4.1750	-1.4097	0.0000	C	4.4278	3.5346	0.0000	H	0.7387	-2.4996	0.0000
C	-4.1776	1.4019	0.0000	C	3.2290	2.8429	0.0000	H	0.7341	2.5008	0.0000
C	-2.9441	0.7097	0.0000	C	4.4202	-0.7259	0.0000	H	6.5751	0.8931	0.0000
C	-2.9427	-0.7153	0.0000	C	3.2068	-1.4340	0.0000	H	6.5832	3.3779	0.0000
C	-1.7165	-1.4075	0.0000	C	3.2345	-2.8369	0.0000	H	4.4302	4.6294	0.0000
C	-1.7191	1.4042	0.0000	C	4.4347	-3.5263	0.0000	H	2.2749	3.3920	0.0000
C	-0.5147	0.7133	0.0000	C	5.6387	-2.8232	0.0000	H	2.2816	-3.3880	0.0000
C	-0.5134	-0.7144	0.0000	C	5.6283	-1.4392	0.0000	H	4.4393	-4.6211	0.0000
C	0.7429	-1.3974	0.0000	H	-8.7678	1.2287	0.0000	H	6.5898	-3.3653	0.0000
C	0.7403	1.3987	0.0000	H	-8.7655	-1.2448	0.0000	H	6.5768	-0.8806	0.0000

Table 3.472: Table of thermodynamic data as a function of temperature for Dibenzo[*a,c*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.410	530.398	530.398	∞
100	127.476	374.375	869.462	-49.509	559.832	615.904	-321.709
200	247.578	497.499	652.800	-31.060	544.254	678.188	-177.121
250	317.615	560.210	627.984	-16.943	536.927	712.519	-148.870
298.15	386.003	622.013	622.013	0.000	530.398	746.947	-130.859
300	388.600	624.409	622.021	0.717	530.158	748.289	-130.286
350	456.939	689.496	627.005	21.872	524.142	785.133	-117.172
400	520.380	754.715	638.895	46.328	518.925	822.773	-107.441
450	577.907	819.388	655.364	73.811	514.419	861.030	-99.944
500	629.377	882.993	674.958	104.018	510.528	899.778	-93.997
600	715.805	1005.692	719.947	171.447	504.256	978.251	-85.163
700	784.286	1121.376	769.117	246.581	499.758	1057.636	-78.920
800	839.315	1229.823	820.002	327.857	496.828	1137.538	-74.272
900	884.243	1331.361	871.240	414.108	495.263	1217.718	-70.673
1000	921.419	1426.509	922.061	504.448	494.877	1298.022	-67.800
1100	952.509	1515.830	972.022	598.190	495.447	1378.326	-65.450
1200	978.727	1599.865	1020.875	694.788	496.813	1458.523	-63.487
1300	1000.994	1679.108	1068.490	793.804	498.770	1538.593	-61.820
1400	1020.020	1754.004	1114.805	894.879	501.169	1618.499	-60.386
1500	1036.370	1824.950	1159.804	997.719	503.917	1698.223	-59.136
1600	1050.493	1892.298	1203.498	1102.079	506.868	1777.746	-58.036
1700	1062.754	1956.360	1245.916	1207.755	509.939	1857.053	-57.059
1800	1073.449	2017.415	1287.094	1314.577	513.045	1936.249	-56.187
1900	1082.821	2075.710	1327.078	1422.401	516.150	2015.215	-55.401
2000	1091.069	2131.465	1365.913	1531.104	519.194	2094.047	-54.690
2100	1098.358	2184.879	1403.649	1640.583	522.088	2172.714	-54.042
2200	1104.826	2236.127	1440.332	1750.748	524.833	2251.251	-53.450
2300	1110.586	2285.368	1476.009	1861.524	527.420	2329.664	-52.907
2400	1115.736	2332.745	1510.726	1972.845	529.772	2407.917	-52.406
2500	1120.354	2378.386	1544.525	2084.654	531.900	2486.202	-51.945
2600	1124.511	2422.410	1577.448	2196.901	533.765	2564.277	-51.516
2700	1128.264	2464.921	1609.535	2309.543	535.371	2642.365	-51.119
2800	1131.661	2506.016	1640.822	2422.542	536.689	2720.424	-50.749
2900	1134.747	2545.782	1671.346	2535.865	537.686	2798.382	-50.403
3000	1137.556	2584.299	1701.139	2649.482	538.410	2876.339	-50.080
3100	1140.120	2621.642	1730.233	2763.368	538.776	2954.193	-49.777
3200	1142.466	2657.877	1758.659	2877.499	538.829	3032.121	-49.493
3300	1144.618	2693.066	1786.444	2991.854	538.549	3110.097	-49.228
3400	1146.596	2727.266	1813.614	3106.416	537.905	3187.990	-48.976
3500	1148.419	2760.530	1840.196	3221.168	536.902	3265.888	-48.740
3600	1150.101	2792.906	1866.212	3336.095	535.564	3343.914	-48.518
3700	1151.657	2824.439	1891.686	3451.184	533.857	3422.004	-48.309
3800	1153.098	2855.171	1916.638	3566.423	531.750	3500.076	-48.111
3900	1154.436	2885.141	1941.089	3681.801	529.291	3578.153	-47.923
4000	1155.681	2914.384	1965.057	3797.307	526.460	3656.451	-47.747
4100	1156.839	2942.935	1988.561	3912.934	523.217	3734.741	-47.580
4200	1157.920	2970.826	2011.618	4028.672	519.595	3813.107	-47.422
4300	1158.930	2998.084	2034.243	4144.515	515.576	3891.463	-47.271
4400	1159.875	3024.738	2056.453	4260.456	511.172	3970.020	-47.129
4500	1160.759	3050.814	2078.261	4376.488	506.397	4048.744	-46.996
4600	1161.590	3076.335	2099.682	4492.606	501.195	4127.585	-46.869
4700	1162.369	3101.325	2120.728	4608.805	495.581	4206.419	-46.748
4800	1163.103	3125.805	2141.413	4725.079	489.608	4285.493	-46.635
4900	1163.793	3149.794	2161.748	4841.424	483.193	4364.546	-46.526
5000	1164.444	3173.313	2181.745	4957.836	476.440	4443.943	-46.425

3.473. Benzo[*a*]naphtho[1,2-*c*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-45-0
Point Group: C₁

Length: 18.23 Å
Width: 11.39 Å
Breadth: 5.149 Å
L/B Ratio: 1.601

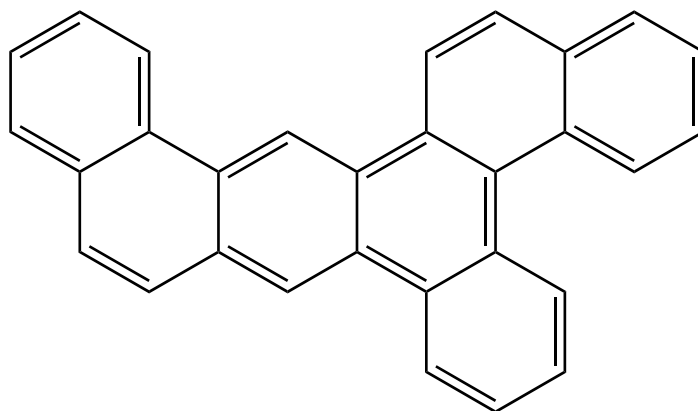
Cartesian coordinates:

C	-3.8467	-1.1847	-0.3080	C	2.8326	2.8498	0.5115	H	-1.5581	-2.6062	-0.3515
C	-3.4778	1.5491	0.2289	C	1.5964	2.2831	0.5538	H	-0.9086	2.2709	0.5162
C	-2.3639	0.6997	0.1520	C	3.9528	2.0694	0.1142	H	-5.7614	2.9644	0.3257
C	-2.5511	-0.6822	-0.1165	C	3.7966	0.6877	-0.1337	H	-8.0438	2.0409	-0.0179
C	-1.4107	-1.5291	-0.1714	C	4.9123	0.0014	-0.6856	H	-8.3683	-0.3654	-0.4941
C	-1.0421	1.1941	0.3251	C	6.1119	0.6294	-0.8945	H	-6.4174	-1.8997	-0.6361
C	-4.9495	-0.3386	-0.2332	C	6.2756	1.9899	-0.5628	H	2.9757	3.9116	0.7421
C	-4.7625	1.0474	0.0405	C	5.2110	2.6984	-0.0748	H	0.7132	2.8961	0.7889
C	-5.9150	1.9001	0.1146	C	2.3176	-1.3818	0.1617	H	4.8089	-1.0570	-0.9614
C	-7.1617	1.3947	-0.0733	C	1.0188	-1.9160	0.0544	H	6.9545	0.0797	-1.3271
C	-7.3489	0.0065	-0.3480	C	0.8326	-3.3080	0.0591	H	7.2484	2.4689	-0.7124
C	-6.2836	-0.8325	-0.4258	C	1.8983	-4.1693	0.2380	H	5.3107	3.7631	0.1664
C	0.0538	0.3666	0.2433	C	3.1736	-3.6445	0.4430	H	-0.1851	-3.7075	-0.0702
C	-0.1415	-1.0354	0.0164	C	3.3733	-2.2761	0.4080	H	1.7414	-5.2526	0.2375
C	1.4143	0.8918	0.3117	H	-3.9884	-2.2521	-0.5171	H	4.0170	-4.3162	0.6340
C	2.5176	0.0673	0.1068	H	-3.3323	2.6161	0.4378	H	4.3870	-1.8886	0.5794

Table 3.473: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[1,2-*c*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.200	534.682	534.682	∞
100	126.751	376.401	870.773	-49.437	564.187	620.057	-323.878
200	247.207	499.188	654.366	-31.036	548.562	682.158	-178.158
250	317.358	561.828	629.566	-16.935	541.219	716.407	-149.682
298.15	385.904	623.599	623.599	0.000	534.682	750.758	-131.527
300	388.508	625.994	623.606	0.716	534.441	752.097	-130.949
350	457.018	691.079	628.590	21.871	528.425	788.862	-117.729
400	520.603	756.319	640.481	46.335	523.216	826.422	-107.917
450	578.235	821.025	656.954	73.832	518.724	864.598	-100.358
500	629.772	884.668	676.554	104.057	514.851	903.263	-94.361
600	716.252	1007.445	721.563	171.529	508.622	981.565	-85.451
700	784.718	1123.197	770.758	246.707	504.168	1060.771	-79.154
800	839.705	1231.700	821.668	328.025	501.279	1140.489	-74.465
900	884.584	1333.280	872.933	414.313	499.750	1220.479	-70.833
1000	921.713	1428.462	923.777	504.684	499.396	1300.588	-67.934
1100	952.761	1517.809	973.761	598.453	499.994	1380.696	-65.562
1200	978.944	1601.865	1022.636	695.075	501.383	1460.694	-63.581
1300	1001.180	1681.124	1070.270	794.110	503.360	1540.563	-61.899
1400	1020.181	1756.033	1116.602	895.203	505.777	1620.267	-60.452
1500	1036.510	1826.989	1161.617	998.058	508.540	1699.788	-59.191
1600	1050.616	1894.345	1205.325	1102.431	511.504	1779.106	-58.081
1700	1062.862	1958.414	1247.756	1208.119	514.586	1858.208	-57.095
1800	1073.544	2019.475	1288.946	1314.951	517.702	1937.199	-56.215
1900	1082.906	2077.774	1328.941	1422.784	520.817	2015.958	-55.421
2000	1091.145	2133.534	1367.787	1531.495	523.868	2094.584	-54.704
2100	1098.426	2186.951	1405.532	1640.981	526.770	2173.044	-54.050
2200	1104.887	2238.202	1442.223	1751.153	529.521	2251.373	-53.453
2300	1110.642	2287.445	1477.909	1861.935	532.114	2329.579	-52.905
2400	1115.787	2334.825	1512.633	1973.261	534.471	2407.624	-52.399
2500	1120.401	2380.469	1546.439	2085.074	536.604	2485.700	-51.935
2600	1124.554	2424.494	1579.368	2197.326	538.474	2563.567	-51.502
2700	1128.303	2467.006	1611.461	2309.972	540.084	2641.447	-51.101
2800	1131.698	2508.102	1642.754	2422.975	541.406	2719.298	-50.728
2900	1134.780	2547.870	1673.283	2536.301	542.406	2797.046	-50.379
3000	1137.587	2586.389	1703.081	2649.922	543.133	2874.794	-50.054
3100	1140.149	2623.732	1732.181	2763.810	543.502	2952.440	-49.747
3200	1142.493	2659.968	1760.611	2877.944	543.558	3030.159	-49.461
3300	1144.644	2695.158	1788.400	2992.302	543.280	3107.925	-49.193
3400	1146.620	2729.359	1815.574	3106.867	542.639	3185.609	-48.940
3500	1148.441	2762.623	1842.160	3221.621	541.638	3263.298	-48.701
3600	1150.122	2795.000	1868.180	3336.551	540.302	3341.115	-48.477
3700	1151.677	2826.533	1893.657	3451.642	538.597	3418.995	-48.267
3800	1153.117	2857.266	1918.613	3566.882	536.493	3496.857	-48.067
3900	1154.454	2887.236	1943.066	3682.262	534.035	3574.725	-47.877
4000	1155.698	2916.480	1967.038	3797.770	531.206	3652.813	-47.700
4100	1156.855	2945.032	1990.544	3913.398	527.965	3730.894	-47.531
4200	1157.935	2972.922	2013.604	4029.138	524.344	3809.050	-47.371
4300	1158.944	3000.181	2036.231	4144.983	520.327	3887.197	-47.219
4400	1159.888	3026.835	2058.443	4260.925	515.924	3965.544	-47.076
4500	1160.773	3052.911	2080.254	4376.959	511.151	4044.058	-46.941
4600	1161.602	3078.433	2101.677	4493.078	505.950	4122.690	-46.814
4700	1162.381	3103.423	2122.726	4609.277	500.337	4201.313	-46.691
4800	1163.114	3127.903	2143.413	4725.553	494.365	4280.178	-46.577
4900	1163.804	3151.893	2163.750	4841.899	487.952	4359.021	-46.467
5000	1164.455	3175.411	2183.749	4958.312	481.200	4438.208	-46.365

3.474. Benzo[*p*]naphtho[2,1-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-56-3
Point Group: C₁

Length: 16.43 Å
Width: 11.76 Å
Breadth: 5.037 Å
L/B Ratio: 1.397

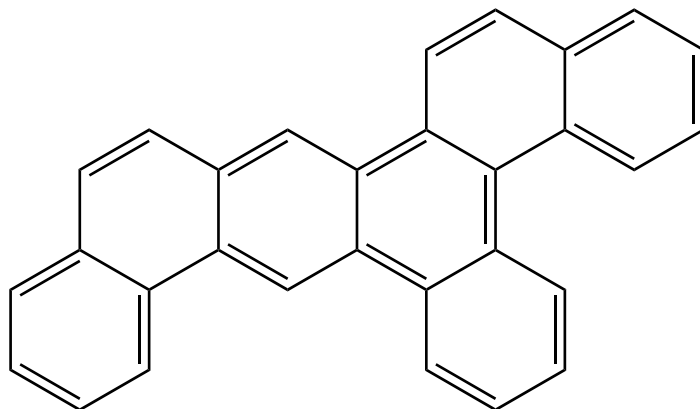
Cartesian coordinates:

C	6.3864	-1.9523	-0.0455	C	-2.1532	-2.9076	-0.4587	H	3.0531	-2.6220	-0.3858
C	6.3240	-0.5927	0.1712	C	-1.0191	-2.1581	-0.4633	H	5.2706	-3.7690	-0.4180
C	3.9855	-2.0577	-0.2301	C	-2.3099	1.3562	-0.1702	H	5.9459	2.0330	0.5740
C	5.2097	-2.6893	-0.2472	C	-1.1092	2.0817	-0.0417	H	3.7603	3.2104	0.6086
C	3.8990	-0.6682	-0.0110	C	-1.1345	3.4884	-0.0617	H	1.3296	3.1657	0.3888
C	5.0791	0.0681	0.1915	C	-2.3106	4.1759	-0.2772	H	1.4600	-1.7667	-0.3378
C	5.0078	1.4880	0.4178	C	-3.4894	3.4615	-0.5042	H	-2.1222	-3.9819	-0.6730
C	3.8176	2.1294	0.4367	C	-3.4832	2.0817	-0.4538	H	-0.0421	-2.6293	-0.6501
C	2.6212	0.0156	0.0105	C	-3.3973	-2.3038	-0.1214	H	-0.1912	4.0367	0.0852
C	2.5878	1.4098	0.2307	C	-3.4665	-0.9122	0.1083	H	-2.3208	5.2704	-0.2894
C	1.3579	2.0747	0.2366	C	-4.6939	-0.4023	0.6095	H	-4.4177	3.9984	-0.7255
C	1.4187	-0.6730	-0.1746	C	-5.7903	-1.2066	0.7834	H	-4.4217	1.5437	-0.6456
C	0.1888	-0.0167	-0.1478	C	-5.7294	-2.5781	0.4659	H	-4.7660	0.6610	0.8761
C	0.1631	1.3848	0.0381	C	-4.5489	-3.1180	0.0296	H	-6.7232	-0.7895	1.1770
C	-1.0641	-0.7504	-0.2444	H	7.3537	-2.4649	-0.0612	H	-6.6218	-3.2006	0.5856
C	-2.2894	-0.1023	-0.0970	H	7.2408	-0.0134	0.3295	H	-4.4734	-4.1876	-0.1977

Table 3.474: Table of thermodynamic data as a function of temperature for Benzo[*p*]naphtho[2,1-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.140	510.023	510.023	∞
100	127.010	375.726	869.476	-49.375	539.590	595.528	-311.065
200	246.849	498.506	653.396	-30.978	523.961	657.693	-171.768
250	316.751	561.037	628.644	-16.902	516.593	691.979	-144.578
298.15	385.161	622.688	622.688	0.000	510.023	726.370	-127.254
300	387.761	625.078	622.695	0.715	509.781	727.711	-126.703
350	456.225	690.044	627.669	21.831	503.726	764.526	-114.097
400	519.823	755.178	639.539	46.256	498.478	802.140	-104.747
450	577.497	819.795	655.985	73.714	493.947	840.375	-97.546
500	629.086	883.362	675.555	103.904	490.039	879.104	-91.837
600	715.665	1006.024	720.503	171.313	483.747	957.542	-83.360
700	784.209	1121.691	769.640	246.436	479.238	1036.895	-77.372
800	839.255	1230.130	820.498	327.706	476.301	1116.766	-72.916
900	884.178	1331.660	871.715	413.951	474.730	1196.916	-69.466
1000	921.344	1426.801	922.517	504.284	474.337	1277.190	-66.712
1100	952.422	1516.115	972.463	598.017	474.899	1357.466	-64.459
1200	978.632	1600.142	1021.303	694.606	476.256	1437.634	-62.577
1300	1000.892	1679.377	1068.906	793.612	478.203	1517.677	-60.980
1400	1019.916	1754.265	1115.210	894.677	480.592	1597.556	-59.604
1500	1036.265	1825.204	1160.200	997.506	483.329	1677.255	-58.406
1600	1050.389	1892.545	1203.885	1101.856	486.270	1756.752	-57.351
1700	1062.652	1956.601	1246.294	1207.522	489.330	1836.035	-56.413
1800	1073.350	2017.650	1287.464	1314.334	492.426	1915.208	-55.577
1900	1082.725	2075.939	1327.440	1422.148	495.522	1994.150	-54.822
2000	1090.977	2131.690	1366.269	1530.842	498.556	2072.959	-54.139
2100	1098.270	2185.099	1403.999	1640.311	501.441	2151.604	-53.517
2200	1104.742	2236.343	1440.676	1750.468	504.177	2230.119	-52.949
2300	1110.506	2285.580	1476.347	1861.236	506.756	2308.511	-52.427
2400	1115.659	2332.954	1511.058	1972.549	509.100	2386.743	-51.945
2500	1120.282	2378.593	1544.853	2084.350	511.221	2465.007	-51.502
2600	1124.442	2422.613	1577.771	2196.590	513.079	2543.062	-51.090
2700	1128.198	2465.122	1609.853	2309.225	514.678	2621.130	-50.708
2800	1131.599	2506.214	1641.136	2422.218	515.990	2699.169	-50.353
2900	1134.687	2545.978	1671.656	2535.535	516.981	2777.106	-50.020
3000	1137.499	2584.494	1701.445	2649.146	517.699	2855.044	-49.710
3100	1140.066	2621.835	1730.536	2763.026	518.059	2932.879	-49.418
3200	1142.415	2658.068	1758.958	2877.152	518.107	3010.788	-49.145
3300	1144.569	2693.256	1786.740	2991.503	517.822	3088.744	-48.890
3400	1146.550	2727.454	1813.907	3106.060	517.173	3166.619	-48.648
3500	1148.374	2760.717	1840.486	3220.808	516.166	3244.498	-48.420
3600	1150.058	2793.091	1866.500	3335.730	514.823	3322.506	-48.207
3700	1151.616	2824.623	1891.970	3450.815	513.112	3400.577	-48.007
3800	1153.059	2855.354	1916.920	3566.050	511.002	3478.630	-47.816
3900	1154.399	2885.323	1941.368	3681.423	508.539	3556.689	-47.636
4000	1155.645	2914.566	1965.334	3796.926	505.704	3634.969	-47.467
4100	1156.805	2943.116	1988.836	3912.550	502.458	3713.241	-47.306
4200	1157.887	2971.005	2011.890	4028.285	498.832	3791.588	-47.154
4300	1158.898	2998.263	2034.513	4144.125	494.810	3869.927	-47.009
4400	1159.844	3024.916	2056.721	4260.062	490.402	3948.466	-46.873
4500	1160.730	3050.992	2078.527	4376.092	485.625	4027.172	-46.745
4600	1161.562	3076.512	2099.946	4492.207	480.420	4105.996	-46.624
4700	1162.342	3101.502	2120.990	4608.402	474.803	4184.812	-46.508
4800	1163.077	3125.981	2141.674	4724.674	468.828	4263.868	-46.399
4900	1163.768	3149.970	2162.007	4841.016	462.410	4342.904	-46.295
5000	1164.420	3173.487	2182.002	4957.426	455.655	4422.283	-46.198

3.475. Benzo[*p*]naphtho[1,2-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-55-2
Point Group: C₁

Length: 17.87 Å
Width: 11.15 Å
Breadth: 5.174 Å
L/B Ratio: 1.604

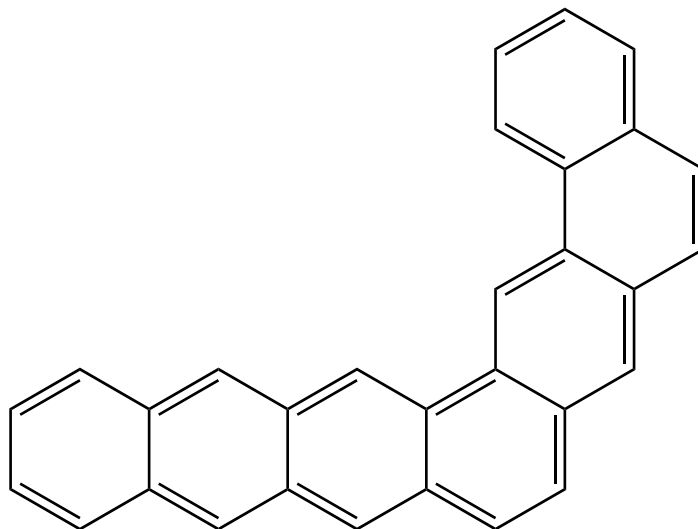
Cartesian coordinates:

C	-6.4001	0.8001	-0.2319	C	3.2574	2.6587	0.4249	H	-6.3580	-2.5731	-0.6408
C	-6.8695	-0.4810	-0.4267	C	1.9371	2.3410	0.4868	H	-3.9038	-2.1786	-0.3931
C	-5.9740	-1.5595	-0.4859	C	4.2058	1.6661	0.0494	H	-2.8152	3.6241	0.4031
C	-4.6202	-1.3438	-0.3499	C	3.7870	0.3337	-0.1588	H	-5.2470	3.1924	0.1569
C	-5.0178	1.0374	-0.0910	C	4.7447	-0.5657	-0.6987	H	-2.1277	-1.8690	-0.1817
C	-4.1191	-0.0417	-0.1508	C	6.0411	-0.1841	-0.9291	H	-0.5249	2.8103	0.4600
C	-3.1957	2.6080	0.2477	C	6.4645	1.1269	-0.6336	H	3.6032	3.6798	0.6222
C	-4.5205	2.3728	0.1135	C	5.5583	2.0384	-0.1609	H	1.1884	3.1177	0.7043
C	-2.2439	1.5290	0.1893	C	1.9408	-1.4037	0.2049	H	4.4390	-1.5906	-0.9493
C	-2.6989	0.2069	-0.0063	C	0.5606	-1.6768	0.1361	H	6.7586	-0.8956	-1.3512
C	-1.7648	-0.8320	-0.0465	C	0.1056	-3.0076	0.1804	H	7.5095	1.4077	-0.7990
C	-0.8732	1.7751	0.3163	C	0.9853	-4.0542	0.3622	H	5.8615	3.0704	0.0502
C	0.0592	0.7394	0.2546	C	2.3455	-3.7839	0.5297	H	-0.9736	-3.2012	0.0804
C	-0.4002	-0.5881	0.0932	C	2.8077	-2.4849	0.4552	H	0.6224	-5.0865	0.3936
C	1.4902	1.0019	0.2901	H	-7.0964	1.6451	-0.1846	H	3.0441	-4.6044	0.7236
C	2.4143	-0.0256	0.1066	H	-7.9433	-0.6645	-0.5363	H	3.8807	-2.2990	0.6004

Table 3.475: Table of thermodynamic data as a function of temperature for Benzo[*p*]naphtho[1,2-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.003	510.016	510.016	∞
100	126.564	374.597	867.362	-49.277	539.681	595.732	-311.172
200	246.355	497.058	651.687	-30.926	524.006	658.028	-171.856
250	316.216	559.474	626.975	-16.875	516.613	692.389	-144.664
298.15	384.596	621.028	621.028	0.000	510.016	726.858	-127.340
300	387.196	623.415	621.035	0.714	509.773	728.202	-126.789
350	455.646	688.293	626.003	21.801	503.689	765.102	-114.183
400	519.247	753.350	637.857	46.197	498.412	802.806	-104.833
450	576.937	817.899	654.283	73.627	493.853	841.134	-97.634
500	628.552	881.409	673.831	103.789	489.917	879.959	-91.927
600	715.191	1003.978	718.732	171.148	483.575	958.598	-83.452
700	783.797	1119.577	767.825	246.227	479.022	1038.158	-77.467
800	838.898	1227.965	818.642	327.458	476.046	1118.244	-73.012
900	883.869	1329.456	869.822	413.670	474.442	1198.612	-69.564
1000	921.074	1424.566	920.592	503.974	474.020	1279.108	-66.812
1100	952.186	1513.856	970.508	597.682	474.557	1359.608	-64.561
1200	978.424	1597.863	1019.323	694.249	475.892	1440.004	-62.680
1300	1000.708	1677.083	1066.902	793.235	477.819	1520.275	-61.084
1400	1019.752	1751.958	1113.185	894.283	480.191	1600.385	-59.710
1500	1036.118	1822.886	1158.155	997.096	482.912	1680.314	-58.513
1600	1050.257	1890.218	1201.823	1101.432	485.839	1760.044	-57.458
1700	1062.532	1954.266	1244.216	1207.086	488.887	1839.560	-56.522
1800	1073.241	2015.309	1285.372	1313.886	491.971	1918.967	-55.686
1900	1082.626	2073.593	1325.335	1421.690	495.057	1998.143	-54.932
2000	1090.886	2129.339	1364.152	1530.374	498.081	2077.187	-54.249
2100	1098.187	2182.744	1401.870	1639.835	500.958	2156.068	-53.628
2200	1104.665	2233.984	1438.536	1749.984	503.686	2234.818	-53.060
2300	1110.436	2283.218	1474.198	1860.745	506.258	2313.446	-52.539
2400	1115.594	2330.589	1508.901	1972.051	508.595	2391.914	-52.058
2500	1120.221	2376.225	1542.686	2083.846	510.710	2470.415	-51.615
2600	1124.386	2420.243	1575.597	2196.080	512.562	2548.707	-51.203
2700	1128.146	2462.750	1607.672	2308.710	514.156	2627.012	-50.822
2800	1131.550	2503.840	1638.948	2421.697	515.462	2705.288	-50.467
2900	1134.641	2543.603	1669.461	2535.009	516.448	2783.463	-50.135
3000	1137.456	2582.117	1699.245	2648.616	517.162	2861.639	-49.825
3100	1140.025	2619.456	1728.330	2762.492	517.518	2939.711	-49.533
3200	1142.377	2655.688	1756.746	2876.614	517.562	3017.858	-49.260
3300	1144.533	2690.875	1784.523	2990.961	517.273	3096.053	-49.005
3400	1146.516	2725.072	1811.685	3105.515	516.621	3174.165	-48.764
3500	1148.342	2758.334	1838.260	3220.259	515.610	3252.282	-48.537
3600	1150.028	2790.707	1864.269	3335.179	514.265	3330.529	-48.324
3700	1151.587	2822.238	1889.736	3450.260	512.550	3408.838	-48.123
3800	1153.032	2852.969	1914.681	3565.492	510.437	3487.130	-47.933
3900	1154.373	2882.937	1939.126	3680.863	507.971	3565.428	-47.753
4000	1155.620	2912.179	1963.088	3796.364	505.134	3643.946	-47.584
4100	1156.781	2940.729	1986.586	3911.984	501.885	3722.457	-47.424
4200	1157.865	2968.617	2009.637	4027.717	498.257	3801.043	-47.272
4300	1158.877	2995.874	2032.257	4143.555	494.233	3879.621	-47.127
4400	1159.824	3022.527	2054.461	4259.491	489.823	3958.399	-46.991
4500	1160.711	3048.602	2076.265	4375.518	485.044	4037.343	-46.863
4600	1161.543	3074.122	2097.681	4491.631	479.837	4116.406	-46.742
4700	1162.324	3099.111	2118.723	4607.825	474.218	4195.461	-46.626
4800	1163.059	3123.590	2139.404	4724.094	468.241	4274.757	-46.518
4900	1163.751	3147.579	2159.735	4840.435	461.822	4354.031	-46.414
5000	1164.404	3171.096	2179.728	4956.843	455.065	4433.649	-46.317

3.476. Benzo[*a*]hexaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-79-0
Point Group: C_s

Length: 18.18 Å
Width: 11.32 Å
Breadth: 3.887 Å
L/B Ratio: 1.606

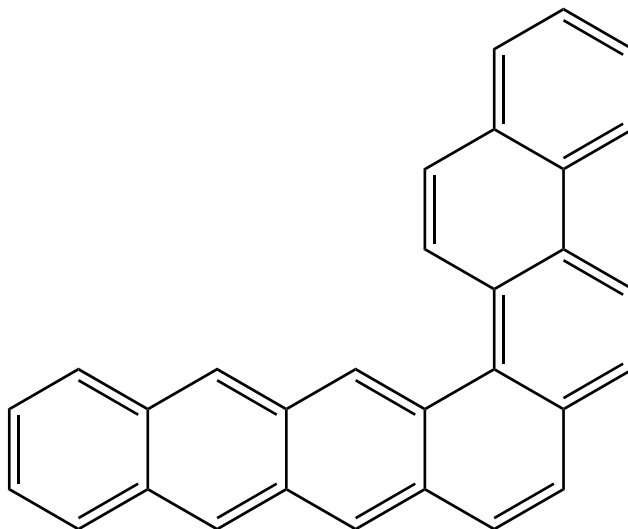
Cartesian coordinates:

C	6.6973	-2.5791	0.0000	C	-1.0425	1.1636	0.0000	H	7.3153	0.7887	0.0000
C	7.4228	-1.3497	0.0000	C	-1.7046	2.4162	0.0000	H	4.7735	-3.5188	0.0000
C	6.7670	-0.1602	0.0000	C	-3.0938	2.4652	0.0000	H	5.2002	2.0380	0.0000
C	5.3390	-2.5801	0.0000	C	-1.7962	-0.0038	0.0000	H	2.6572	-2.2710	0.0000
C	4.6079	-1.3447	0.0000	C	-3.1972	0.0352	0.0000	H	3.0860	3.2832	0.0000
C	5.3321	-0.1174	0.0000	C	-3.8516	1.2850	0.0000	H	0.5334	-1.0205	0.0000
C	4.6441	1.0924	0.0000	C	-5.2897	1.3358	0.0000	H	1.0045	4.5346	0.0000
C	3.2162	-1.3272	0.0000	C	-6.0246	0.2001	0.0000	H	-1.4710	4.5882	0.0000
C	2.5189	-0.1097	0.0000	C	-3.9866	-1.1791	0.0000	H	-3.6066	3.4352	0.0000
C	3.2412	1.1147	0.0000	C	-5.3894	-1.0906	0.0000	H	-1.2846	-0.9857	0.0000
C	2.5217	2.3422	0.0000	C	-6.1613	-2.2708	0.0000	H	-5.7714	2.3204	0.0000
C	1.0973	-0.0734	0.0000	C	-5.5467	-3.5036	0.0000	H	-7.1202	0.2362	0.0000
C	0.4157	1.1200	0.0000	C	-4.1460	-3.5943	0.0000	H	-7.2547	-2.1953	0.0000
C	1.1474	2.3547	0.0000	C	-3.3783	-2.4511	0.0000	H	-6.1465	-4.4196	0.0000
C	0.4194	3.6074	0.0000	H	7.2594	-3.5187	0.0000	H	-3.6684	-4.5795	0.0000
C	-0.9261	3.6370	0.0000	H	8.5170	-1.3875	0.0000	H	-2.2786	-2.5044	0.0000

Table 3.476: Table of thermodynamic data as a function of temperature for Benzo[*a*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.211	502.134	502.134	∞
100	125.965	378.880	873.259	-49.438	531.638	587.260	-306.747
200	247.293	501.354	656.735	-31.076	515.974	649.137	-169.534
250	317.807	564.055	631.900	-16.961	508.645	683.276	-142.760
298.15	386.533	625.922	625.922	0.000	502.134	717.517	-125.703
300	389.141	628.321	625.930	0.717	501.894	718.852	-125.161
350	457.698	693.509	630.921	21.906	495.912	755.498	-112.750
400	521.255	758.838	642.830	46.403	490.736	792.934	-103.544
450	578.830	823.618	659.327	73.931	486.275	830.982	-96.456
500	630.306	887.320	678.952	104.184	482.430	869.517	-90.836
600	716.695	1010.186	724.011	171.705	476.250	947.548	-82.490
700	785.121	1126.003	773.253	246.925	471.838	1026.477	-76.595
800	840.097	1234.559	824.206	328.282	468.988	1105.911	-72.207
900	884.978	1336.185	875.508	414.609	467.499	1185.613	-68.810
1000	922.110	1431.409	926.388	505.021	467.184	1265.430	-66.098
1100	953.157	1520.794	976.404	598.829	467.822	1345.241	-63.879
1200	979.334	1604.884	1025.309	695.490	469.251	1424.939	-62.025
1300	1001.561	1684.174	1072.970	794.564	471.266	1504.504	-60.450
1400	1020.549	1759.110	1119.329	895.694	473.720	1583.902	-59.095
1500	1036.862	1830.091	1164.368	998.585	476.519	1663.113	-57.914
1600	1050.952	1897.469	1208.099	1102.993	479.518	1742.120	-56.873
1700	1063.181	1961.558	1250.551	1208.714	482.633	1820.909	-55.949
1800	1073.846	2022.637	1291.761	1315.577	485.780	1899.585	-55.123
1900	1083.191	2080.953	1331.774	1423.439	488.924	1978.027	-54.379
2000	1091.414	2136.727	1370.638	1532.178	492.003	2056.333	-53.705
2100	1098.680	2190.156	1408.399	1641.690	494.931	2134.474	-53.091
2200	1105.126	2241.419	1445.107	1751.886	497.706	2212.482	-52.530
2300	1110.868	2290.672	1480.807	1862.691	500.322	2290.365	-52.015
2400	1115.999	2338.061	1515.545	1974.040	502.701	2368.087	-51.539
2500	1120.602	2383.713	1549.364	2085.874	504.856	2445.840	-51.102
2600	1124.743	2427.746	1582.306	2198.144	506.744	2523.382	-50.694
2700	1128.482	2470.266	1614.410	2310.809	508.373	2600.936	-50.317
2800	1131.867	2511.368	1645.715	2423.829	509.712	2678.460	-49.966
2900	1134.941	2551.141	1676.254	2537.172	510.729	2755.882	-49.638
3000	1137.739	2589.665	1706.063	2650.808	511.472	2833.303	-49.331
3100	1140.293	2627.014	1735.171	2764.712	511.856	2910.620	-49.043
3200	1142.630	2663.254	1763.611	2878.859	511.925	2988.011	-48.773
3300	1144.774	2698.448	1791.408	2993.231	511.661	3065.448	-48.521
3400	1146.744	2732.653	1818.591	3107.808	511.032	3142.804	-48.282
3500	1148.559	2765.920	1845.185	3222.575	510.044	3220.162	-48.057
3600	1150.234	2798.300	1871.213	3337.515	508.719	3297.650	-47.847
3700	1151.784	2829.837	1896.697	3452.617	507.025	3375.200	-47.648
3800	1153.219	2860.572	1921.659	3567.868	504.931	3452.732	-47.460
3900	1154.552	2890.545	1946.120	3683.258	502.484	3530.268	-47.282
4000	1155.791	2919.792	1970.098	3798.776	499.664	3608.026	-47.115
4100	1156.945	2948.345	1993.610	3914.413	496.432	3685.775	-46.956
4200	1158.021	2976.238	2016.676	4030.162	492.820	3763.599	-46.806
4300	1159.026	3003.499	2039.309	4146.015	488.811	3841.415	-46.663
4400	1159.967	3030.155	2061.527	4261.965	484.416	3919.430	-46.529
4500	1160.848	3056.233	2083.342	4378.006	479.650	3997.612	-46.402
4600	1161.675	3081.756	2104.771	4494.133	474.457	4075.911	-46.282
4700	1162.451	3106.748	2125.824	4610.340	468.852	4154.203	-46.168
4800	1163.181	3131.229	2146.516	4726.622	462.887	4232.734	-46.061
4900	1163.869	3155.220	2166.858	4842.974	456.479	4311.245	-45.957
5000	1164.517	3178.740	2186.861	4959.394	449.734	4390.099	-45.862

3.477. Phenanthro[1,2-*a*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-63-2
Point Group: C₁

Length: 18.32 Å
Width: 11.09 Å
Breadth: 5.086 Å
L/B Ratio: 1.653

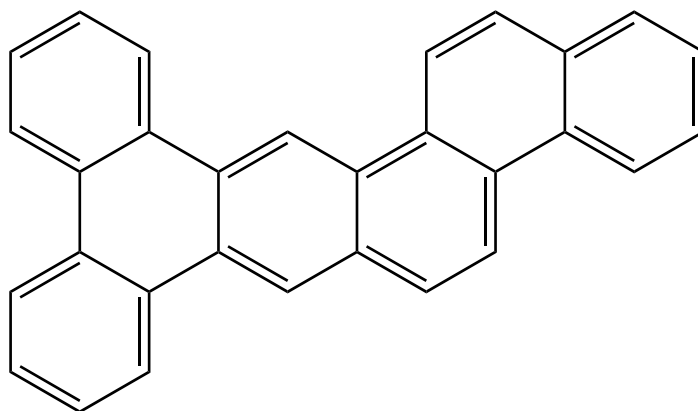
Cartesian coordinates:

C	4.7833	3.1539	0.3875	C	-0.9894	-2.4082	0.2334	H	-7.1304	-0.7189	0.3638
C	3.9153	2.0400	0.3465	C	-0.2222	-1.2040	0.0551	H	-4.5352	3.4289	-0.6776
C	4.3947	0.7916	-0.0833	C	-2.3642	-2.3683	0.3128	H	-5.0369	-2.0031	0.4685
C	5.7526	0.6802	-0.4619	C	-3.0697	-1.1482	0.1604	H	-2.4421	2.1530	-0.5507
C	6.5853	1.7731	-0.4197	C	-2.3303	0.0312	-0.1183	H	-2.9362	-3.2916	0.4703
C	6.0977	3.0211	0.0075	C	-0.9130	-0.0325	-0.1720	H	-0.3764	0.8998	-0.4014
C	3.4961	-0.3406	-0.1279	C	-4.4711	-1.0900	0.2464	H	-0.9202	-4.5873	0.4066
C	2.1292	-0.1788	0.1661	C	-5.1390	0.1127	0.0505	H	1.5159	-4.7300	-0.0525
C	1.7043	1.1003	0.6628	C	-4.3985	1.2960	-0.2441	H	3.5902	-3.7238	-0.5607
C	2.5484	2.1566	0.7542	C	-3.0122	1.2432	-0.3254	H	5.0699	-1.7270	-0.6903
C	4.0031	-1.6255	-0.4392	C	-6.5709	0.1952	0.1350	H	2.2025	3.1192	1.1487
C	3.1868	-2.7193	-0.3871	C	-7.2079	1.3772	-0.0645	H	0.6655	1.2161	1.0016
C	1.8042	-2.5666	-0.1244	C	-6.4667	2.5615	-0.3621	H	6.1291	-0.2999	-0.7916
C	1.2386	-1.2960	0.0369	C	-5.1125	2.5258	-0.4494	H	7.6345	1.6794	-0.7182
C	1.0058	-3.7614	0.0092	H	-7.0155	3.4961	-0.5177	H	6.7733	3.8822	0.0353
C	-0.3176	-3.6863	0.2437	H	-8.2988	1.4455	-0.0014	H	4.3945	4.1211	0.7257

Table 3.477: Table of thermodynamic data as a function of temperature for Phenanthro[1,2-*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.986	531.613	531.613	∞
100	124.966	374.798	868.021	-49.322	561.233	617.263	-322.419
200	246.768	496.729	651.910	-31.036	545.493	679.581	-177.485
250	317.409	559.328	627.103	-16.944	538.141	713.954	-149.169
298.15	386.198	621.132	621.132	0.000	531.613	748.424	-131.118
300	388.808	623.529	621.139	0.717	531.373	749.768	-130.543
350	457.409	688.669	626.127	21.890	525.375	786.655	-117.399
400	521.004	753.962	638.028	46.374	520.186	824.334	-107.645
450	578.611	818.714	654.515	73.890	515.713	862.627	-100.129
500	630.114	882.395	674.129	104.133	511.858	901.407	-94.167
600	716.533	1005.229	719.168	171.636	505.660	979.933	-85.309
700	784.963	1121.021	768.392	246.840	501.232	1059.359	-79.049
800	839.934	1229.555	819.328	328.182	498.367	1139.292	-74.387
900	884.804	1331.162	870.616	414.492	496.861	1219.495	-70.776
1000	921.929	1426.367	921.482	504.885	496.528	1299.815	-67.894
1100	952.971	1515.735	971.485	598.675	497.147	1380.132	-65.536
1200	979.148	1599.808	1020.377	695.317	498.557	1460.336	-63.565
1300	1001.376	1679.083	1068.027	794.373	500.554	1540.410	-61.893
1400	1020.369	1754.006	1114.374	895.485	502.990	1620.317	-60.454
1500	1036.689	1824.975	1159.403	998.358	505.771	1700.040	-59.199
1600	1050.785	1892.342	1203.124	1102.749	508.753	1779.559	-58.095
1700	1063.022	1956.421	1245.567	1208.453	511.851	1858.861	-57.115
1800	1073.696	2017.491	1286.768	1315.301	514.983	1938.050	-56.240
1900	1083.048	2075.799	1326.773	1423.148	518.112	2017.008	-55.450
2000	1091.279	2131.566	1365.629	1531.873	521.177	2095.830	-54.736
2100	1098.552	2184.989	1403.383	1641.372	524.092	2174.487	-54.086
2200	1105.006	2236.245	1440.083	1751.556	526.855	2253.012	-53.492
2300	1110.754	2285.494	1475.777	1862.350	529.460	2331.413	-52.947
2400	1115.892	2332.878	1510.508	1973.687	531.828	2409.653	-52.444
2500	1120.500	2378.526	1544.322	2085.511	533.972	2487.924	-51.981
2600	1124.647	2422.555	1577.258	2197.771	535.850	2565.985	-51.550
2700	1128.391	2465.071	1609.357	2310.427	537.470	2644.059	-51.151
2800	1131.781	2506.170	1640.656	2423.438	538.800	2722.103	-50.780
2900	1134.859	2545.940	1671.191	2536.772	539.808	2800.044	-50.433
3000	1137.662	2584.462	1700.995	2650.401	540.544	2877.985	-50.109
3100	1140.220	2621.808	1730.099	2764.297	540.920	2955.823	-49.804
3200	1142.561	2658.046	1758.534	2878.437	540.982	3033.735	-49.520
3300	1144.708	2693.238	1786.328	2992.802	540.711	3111.693	-49.253
3400	1146.681	2727.440	1813.507	3107.373	540.076	3189.569	-49.001
3500	1148.499	2760.706	1840.097	3222.133	539.081	3267.449	-48.763
3600	1150.177	2793.084	1866.121	3337.068	537.751	3345.458	-48.540
3700	1151.729	2824.619	1891.602	3452.165	536.052	3423.530	-48.331
3800	1153.167	2855.353	1916.561	3567.410	533.952	3501.584	-48.132
3900	1154.502	2885.325	1941.019	3682.795	531.500	3579.642	-47.943
4000	1155.743	2914.570	1964.993	3798.308	528.675	3657.922	-47.767
4100	1156.899	2943.123	1988.503	3913.940	525.438	3736.194	-47.599
4200	1157.977	2971.014	2011.566	4029.685	521.822	3814.540	-47.440
4300	1158.985	2998.274	2034.197	4145.533	517.809	3892.878	-47.288
4400	1159.927	3024.930	2056.412	4261.480	513.410	3971.415	-47.146
4500	1160.810	3051.006	2078.225	4377.517	508.640	4050.120	-47.012
4600	1161.638	3076.529	2099.651	4493.640	503.443	4128.942	-46.885
4700	1162.416	3101.520	2120.702	4609.843	497.834	4207.756	-46.763
4800	1163.147	3126.000	2141.392	4726.121	491.865	4286.811	-46.649
4900	1163.836	3149.991	2161.731	4842.471	485.455	4365.844	-46.540
5000	1164.485	3173.510	2181.733	4958.887	478.706	4445.221	-46.438

3.478. Phenanthro[9,10-*b*]chrysene



Other names: Phenanthro[1,2-*b*]triphenylene

Formula: C₃₀H₁₈

Mass: 378.464 g/mol

CAS Number: 80277-95-8

Point Group: C_s

Length: 17.99 Å

Width: 11.15 Å

Breadth: 3.886 Å

L/B Ratio: 1.614

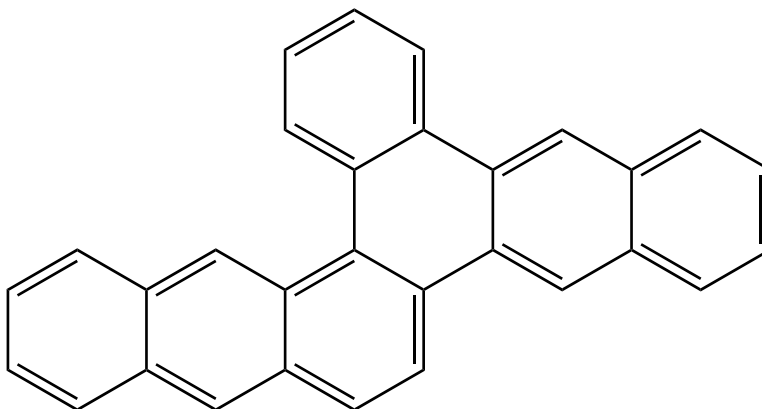
Cartesian coordinates:

C	4.6050	-3.3860	0.0000	C	-0.8469	0.1296	0.0000	H	1.2084	-3.1252	0.0000
C	4.9295	-2.0426	0.0000	C	-0.5074	1.4988	0.0000	H	3.0073	-4.8428	0.0000
C	2.2669	-2.8227	0.0000	C	-1.5473	2.4845	0.0000	H	6.4070	0.0008	0.0000
C	3.2648	-3.7788	0.0000	C	-2.8512	2.1112	0.0000	H	7.0021	2.4153	0.0000
C	2.5793	-1.4526	0.0000	C	-2.2384	-0.2548	0.0000	H	5.2070	4.1397	0.0000
C	3.9274	-1.0576	0.0000	C	-3.2273	0.7286	0.0000	H	2.8180	3.4476	0.0000
C	3.2609	1.3310	0.0000	C	-3.9198	-2.0058	0.0000	H	1.1067	2.9480	0.0000
C	4.2740	0.3577	0.0000	C	-2.6128	-1.6337	0.0000	H	-0.0830	-1.8967	0.0000
C	5.6178	0.7682	0.0000	C	-4.9546	-1.0203	0.0000	H	-1.2638	3.5431	0.0000
C	5.9508	2.1095	0.0000	C	-4.6150	0.3456	0.0000	H	-3.6583	2.8600	0.0000
C	4.9437	3.0771	0.0000	C	-5.6544	1.3078	0.0000	H	-4.2035	-3.0644	0.0000
C	3.6170	2.6903	0.0000	C	-6.9700	0.9178	0.0000	H	-1.8072	-2.3842	0.0000
C	1.5221	-0.4492	0.0000	C	-7.3058	-0.4506	0.0000	H	-5.3795	2.3736	0.0000
C	1.8596	0.9299	0.0000	C	-6.3179	-1.4034	0.0000	H	-7.7692	1.6662	0.0000
C	0.8450	1.8774	0.0000	H	5.3960	-4.1430	0.0000	H	-8.3605	-0.7442	0.0000
C	0.1854	-0.8229	0.0000	H	5.9840	-1.7267	0.0000	H	-6.5702	-2.4699	0.0000

Table 3.478: Table of thermodynamic data as a function of temperature for Phenanthro[9,10-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.281	484.960	484.960	∞
100	127.910	382.057	875.152	-49.310	514.592	569.897	-297.678
200	246.438	504.979	659.476	-30.899	498.977	631.414	-164.905
250	315.929	567.373	634.789	-16.854	491.578	665.380	-139.021
298.15	384.013	628.850	628.850	0.000	484.960	699.470	-122.542
300	386.603	631.234	628.858	0.713	484.716	700.799	-122.017
350	454.823	696.002	633.817	21.765	478.597	737.311	-110.035
400	518.270	760.938	645.651	46.115	473.274	774.632	-101.155
450	575.870	825.366	662.047	73.494	468.664	812.584	-94.320
500	627.443	888.761	681.559	103.601	464.673	851.039	-88.906
600	714.089	1011.127	726.380	170.848	458.219	928.953	-80.871
700	782.758	1126.561	775.389	245.820	453.559	1007.807	-75.202
800	837.939	1234.815	826.126	326.952	450.484	1087.201	-70.985
900	882.991	1336.198	877.229	413.072	448.788	1166.890	-67.723
1000	920.274	1431.220	927.928	503.292	448.282	1246.716	-65.120
1100	951.457	1520.437	977.779	596.924	448.742	1326.555	-62.992
1200	977.760	1604.384	1026.533	693.421	450.008	1406.295	-61.213
1300	1000.102	1683.552	1074.057	792.344	451.872	1485.917	-59.704
1400	1019.199	1758.385	1120.290	893.333	454.185	1565.382	-58.404
1500	1035.612	1829.276	1165.213	996.094	456.854	1644.671	-57.271
1600	1049.793	1896.577	1208.838	1100.381	459.732	1723.763	-56.274
1700	1062.106	1960.598	1251.192	1205.990	462.735	1802.645	-55.387
1800	1072.849	2021.617	1292.312	1312.750	465.779	1881.419	-54.596
1900	1082.265	2079.881	1332.241	1420.516	468.827	1959.966	-53.882
2000	1090.552	2135.609	1371.026	1529.166	471.817	2038.382	-53.236
2100	1097.878	2188.998	1408.715	1638.595	474.662	2116.636	-52.647
2200	1104.378	2240.224	1445.355	1748.714	477.360	2194.762	-52.109
2300	1110.169	2289.446	1480.991	1859.447	479.903	2272.767	-51.615
2400	1115.345	2336.806	1515.670	1970.727	482.215	2350.613	-51.159
2500	1119.989	2382.432	1549.433	2082.498	484.306	2428.492	-50.740
2600	1124.168	2426.442	1582.323	2194.709	486.135	2506.164	-50.348
2700	1127.942	2468.940	1614.378	2307.318	487.708	2583.849	-49.987
2800	1131.359	2510.024	1645.636	2420.286	488.995	2661.507	-49.650
2900	1134.462	2549.780	1676.132	2533.579	489.962	2739.064	-49.335
3000	1137.287	2588.288	1705.898	2647.169	490.659	2816.622	-49.041
3100	1139.866	2625.622	1734.968	2761.028	490.998	2894.078	-48.764
3200	1142.226	2661.849	1763.370	2875.135	491.027	2971.608	-48.506
3300	1144.391	2697.031	1791.132	2989.467	490.723	3049.187	-48.264
3400	1146.381	2731.224	1818.281	3104.007	490.057	3126.684	-48.035
3500	1148.214	2764.482	1844.843	3218.738	489.033	3204.186	-47.819
3600	1149.906	2796.852	1870.840	3333.645	487.675	3281.818	-47.617
3700	1151.471	2828.380	1896.295	3448.715	485.949	3359.513	-47.427
3800	1152.922	2859.107	1921.230	3563.935	483.824	3437.191	-47.247
3900	1154.268	2889.073	1945.663	3679.296	481.348	3514.875	-47.075
4000	1155.520	2918.312	1969.616	3794.786	478.500	3592.779	-46.916
4100	1156.686	2946.859	1993.104	3910.397	475.242	3670.678	-46.764
4200	1157.773	2974.746	2016.146	4026.120	471.604	3748.651	-46.620
4300	1158.789	3002.001	2038.757	4141.949	467.571	3826.615	-46.483
4400	1159.740	3028.652	2060.953	4257.876	463.153	3904.781	-46.355
4500	1160.630	3054.725	2082.748	4373.895	458.365	3983.113	-46.234
4600	1161.466	3080.243	2104.156	4490.000	453.150	4061.564	-46.120
4700	1162.250	3105.231	2125.191	4606.187	447.525	4140.007	-46.010
4800	1162.988	3129.708	2145.864	4722.449	441.540	4218.690	-45.908
4900	1163.683	3153.695	2166.188	4838.783	435.114	4297.353	-45.809
5000	1164.338	3177.211	2186.174	4955.184	428.350	4376.360	-45.719

3.479. Tribenzo[*b,g,k*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-46-1
Point Group: C₁

Length: 18.26 Å
Width: 11.14 Å
Breadth: 5.435 Å
L/B Ratio: 1.639

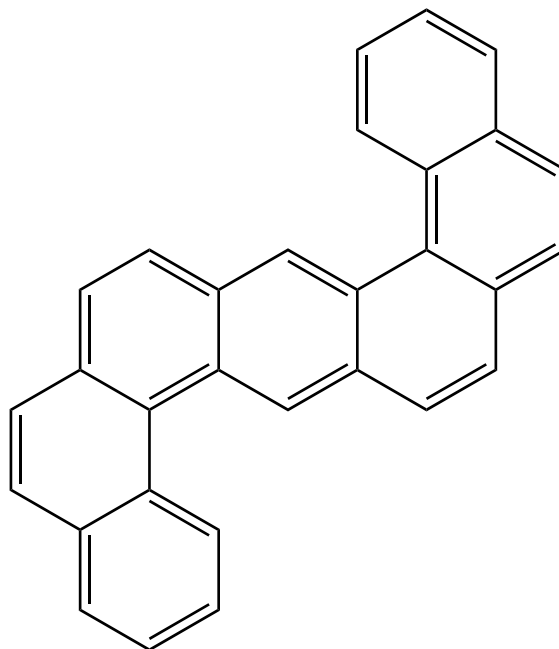
Cartesian coordinates:

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C	6.9157	-0.8247	0.5445	C	-0.7247	4.1971	-0.3486	H	5.0252	1.9573	1.1765
C	5.9541	-1.6773	0.0959	C	0.5984	3.8680	-0.6496	H	3.8147	-3.1502	-0.6627
C	5.2922	0.9389	0.8720	C	1.0032	2.5474	-0.6379	H	2.7030	1.5419	0.6066
C	4.2563	0.0727	0.3961	C	-2.2433	0.7938	0.0144	H	1.4857	-3.6338	-1.0486
C	4.5906	-1.2506	0.0158	C	-1.8602	-0.5567	-0.2175	H	-0.8926	-2.9629	-0.8531
C	3.5719	-2.1123	-0.4023	C	-2.8302	-1.5478	-0.1983	H	-2.6854	3.4307	0.1122
C	2.9303	0.5110	0.2978	C	-3.5649	1.0953	0.3022	H	-1.0405	5.2450	-0.3310
C	1.9123	-0.3193	-0.1735	C	-4.5479	0.0894	0.3455	H	1.3141	4.6587	-0.8977
C	2.2508	-1.6727	-0.4697	C	-4.1770	-1.2479	0.0795	H	2.0482	2.3151	-0.8854
C	1.2095	-2.6080	-0.7789	C	-5.1766	-2.2657	0.1078	H	-2.5488	-2.5946	-0.3940
C	-0.0867	-2.2318	-0.6882	C	-6.4730	-1.9491	0.3922	H	-3.8552	2.1419	0.4874
C	0.5265	0.1029	-0.2968	C	-6.8445	-0.6059	0.6634	H	-4.8811	-3.2999	-0.1016
C	-0.4514	-0.8741	-0.4050	C	-5.9109	0.3890	0.6415	H	-7.2448	-2.7254	0.4159
C	0.1129	1.5035	-0.3229	H	7.3757	1.1590	1.3033	H	-7.8924	-0.3833	0.8899
C	-1.2393	1.8380	-0.1138	H	7.9613	-1.1432	0.6084	H	-6.1882	1.4285	0.8490

Table 3.479: Table of thermodynamic data as a function of temperature for Tribenzo[*b,g,k*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.272	528.873	528.873	∞
100	126.870	376.459	871.309	-49.485	558.330	614.195	-320.816
200	247.459	499.381	654.697	-31.063	542.726	676.284	-176.624
250	317.640	562.080	629.876	-16.949	535.396	710.521	-148.452
298.15	386.212	623.903	623.903	0.000	528.873	744.858	-130.493
300	388.817	626.300	623.911	0.717	528.633	746.197	-129.922
350	457.341	691.434	628.898	21.888	522.633	782.946	-116.846
400	520.929	756.718	640.798	46.368	517.440	820.487	-107.142
450	578.554	821.462	657.282	73.881	512.964	858.642	-99.666
500	630.079	885.138	676.895	104.122	509.107	897.285	-93.737
600	716.523	1007.968	721.930	171.623	502.907	975.536	-84.926
700	784.953	1123.759	771.150	246.826	498.479	1054.688	-78.700
800	839.907	1232.291	822.084	328.166	495.611	1134.348	-74.064
900	884.759	1333.893	873.369	414.472	494.102	1214.278	-70.473
1000	921.865	1429.092	924.232	504.860	493.763	1294.325	-67.607
1100	952.894	1518.454	974.233	598.643	494.375	1374.369	-65.262
1200	979.060	1602.520	1023.122	695.277	495.777	1454.302	-63.303
1300	1001.283	1681.788	1070.769	794.324	497.765	1534.105	-61.640
1400	1020.273	1756.704	1117.114	895.426	500.191	1613.742	-60.208
1500	1036.592	1827.666	1162.139	998.290	502.963	1693.196	-58.961
1600	1050.689	1895.027	1205.858	1102.670	505.935	1772.446	-57.863
1700	1062.929	1959.100	1248.297	1208.366	509.024	1851.480	-56.888
1800	1073.605	2020.165	1289.496	1315.204	512.147	1930.402	-56.018
1900	1082.961	2078.467	1329.498	1423.043	515.267	2009.092	-55.233
2000	1091.195	2134.230	1368.350	1531.759	518.323	2087.648	-54.523
2100	1098.473	2187.649	1406.102	1641.250	521.230	2166.038	-53.876
2200	1104.930	2238.902	1442.799	1751.426	523.986	2244.297	-53.285
2300	1110.681	2288.147	1478.490	1862.212	526.583	2322.433	-52.743
2400	1115.823	2335.528	1513.219	1973.542	528.944	2400.408	-52.242
2500	1120.435	2381.174	1547.030	2085.359	531.081	2478.414	-51.783
2600	1124.585	2425.200	1579.964	2197.614	532.953	2556.211	-51.354
2700	1128.332	2467.714	1612.061	2310.263	534.566	2634.019	-50.957
2800	1131.725	2508.811	1643.358	2423.268	535.891	2711.799	-50.588
2900	1134.806	2548.579	1673.890	2536.597	536.894	2789.477	-50.243
3000	1137.611	2587.099	1703.692	2650.221	537.624	2867.154	-49.921
3100	1140.172	2624.443	1732.794	2764.112	537.995	2944.728	-49.617
3200	1142.515	2660.680	1761.228	2878.248	538.053	3022.377	-49.334
3300	1144.664	2695.870	1789.019	2992.608	537.778	3100.071	-49.069
3400	1146.639	2730.072	1816.197	3107.175	537.138	3177.684	-48.818
3500	1148.459	2763.337	1842.785	3221.931	536.139	3255.301	-48.582
3600	1150.139	2795.714	1868.807	3336.862	534.805	3333.047	-48.360
3700	1151.693	2827.248	1894.287	3451.954	533.102	3410.856	-48.152
3800	1153.133	2857.981	1919.245	3567.197	530.999	3488.647	-47.954
3900	1154.469	2887.951	1943.701	3682.577	528.543	3566.443	-47.766
4000	1155.711	2917.196	1967.674	3798.087	525.715	3644.460	-47.591
4100	1156.869	2945.748	1991.183	3913.717	522.475	3722.469	-47.424
4200	1157.948	2973.638	2014.244	4029.458	518.856	3800.553	-47.266
4300	1158.957	3000.898	2036.873	4145.304	514.840	3878.628	-47.115
4400	1159.900	3027.552	2059.087	4261.248	510.438	3956.904	-46.973
4500	1160.784	3053.629	2080.899	4377.282	505.666	4035.346	-46.840
4600	1161.613	3079.151	2102.324	4493.402	500.466	4113.906	-46.714
4700	1162.392	3104.141	2123.374	4609.603	494.855	4192.458	-46.593
4800	1163.124	3128.621	2144.063	4725.879	488.884	4271.251	-46.480
4900	1163.814	3152.611	2164.401	4842.227	482.471	4350.022	-46.371
5000	1164.464	3176.130	2184.401	4958.641	475.720	4429.137	-46.270

3.480. Dinaphth[1,2-*a*:1',2'-*h*]anthracene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 20495-15-2
Point Group: S₂

Length: 16.92 Å
Width: 10.17 Å
Breadth: 4.722 Å
L/B Ratio: 1.663

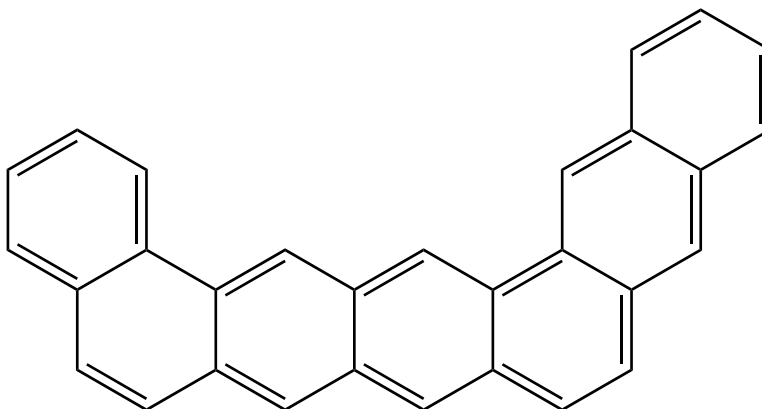
Cartesian coordinates:

C	6.3092	0.7290	-0.2332	C	-1.4071	0.2938	-0.0310	H	4.7052	3.5625	0.6960
C	6.1212	2.0570	0.0506	C	-0.4291	1.2941	-0.2766	H	2.7925	2.0299	0.7492
C	4.8409	2.5125	0.4161	C	-0.8311	2.6613	-0.4573	H	4.6556	-3.5446	-0.2409
C	3.7732	1.6504	0.4319	C	-2.1246	3.0138	-0.2873	H	6.4918	-1.9040	-0.5871
C	5.2217	-0.1779	-0.1875	C	-2.8157	0.6569	-0.0546	H	0.0639	-3.4077	0.6940
C	3.9136	0.2841	0.0779	C	-3.1311	2.0182	-0.0485	H	2.4362	-4.0624	0.3547
C	4.4658	-2.4663	-0.1836	C	-4.4663	2.4661	0.1847	H	1.6394	1.7873	-0.5322
C	5.4729	-1.5727	-0.3563	C	-5.4731	1.5721	0.3571	H	-1.6398	-1.7866	0.5330
C	3.1307	-2.0180	0.0494	C	-3.9135	-0.2841	-0.0783	H	-0.0643	3.4083	-0.6928
C	2.8155	-0.6567	0.0549	C	-5.2217	0.1774	0.1875	H	-2.4367	4.0627	-0.3530
C	0.8306	-2.6608	0.4582	C	-6.3089	-0.7299	0.2326	H	-4.6564	3.5442	0.2426
C	2.1242	-3.0134	0.2885	C	-6.1204	-2.0577	-0.0522	H	-6.4921	1.9031	0.5880
C	0.4289	-1.2936	0.2770	C	-4.8400	-2.5125	-0.4181	H	-7.3054	-0.3504	0.4865
C	1.4069	-0.2935	0.0311	C	-3.7725	-1.6500	-0.4333	H	-6.9564	-2.7634	-0.0167
C	0.9331	0.9833	-0.2779	H	7.3056	0.3490	-0.4870	H	-4.7041	-3.5622	-0.6989
C	-0.9334	-0.9829	0.2782	H	6.9574	2.7625	0.0146	H	-2.7918	-2.0287	-0.7514

Table 3.480: Table of thermodynamic data as a function of temperature for Dinaphth[1,2-*a*:1',2'-*h*]anthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.820	535.285	535.285	∞
100	124.567	368.552	860.122	-49.157	565.070	621.726	-324.749
200	245.888	490.026	644.723	-30.939	549.262	684.690	-178.819
250	316.406	552.414	619.992	-16.894	541.863	719.404	-150.308
298.15	385.168	614.037	614.037	0.000	535.285	754.212	-132.132
300	387.779	616.428	614.045	0.715	535.043	755.569	-131.553
350	456.435	681.413	619.020	21.837	528.995	792.815	-118.319
400	520.123	746.582	630.894	46.275	523.759	830.860	-108.497
450	577.832	811.236	647.348	73.750	519.245	869.524	-100.930
500	629.427	874.839	666.927	103.956	515.353	908.680	-94.927
600	715.984	997.561	711.898	171.398	509.095	987.968	-86.008
700	784.496	1113.276	761.059	246.552	504.616	1068.164	-79.706
800	839.512	1221.751	811.940	327.849	501.706	1148.875	-75.012
900	884.410	1323.310	863.178	414.118	500.160	1229.861	-71.378
1000	921.554	1418.474	914.001	504.473	499.789	1310.969	-68.477
1100	952.614	1507.807	963.964	598.227	500.371	1392.076	-66.103
1200	978.807	1591.850	1012.821	694.834	501.747	1473.075	-64.120
1300	1001.053	1671.099	1060.439	793.857	503.710	1553.946	-62.437
1400	1020.063	1745.998	1106.758	894.937	506.115	1634.653	-60.988
1500	1036.400	1816.946	1151.759	997.781	508.866	1715.177	-59.727
1600	1050.513	1884.296	1195.456	1102.143	511.820	1795.500	-58.616
1700	1062.767	1948.359	1237.876	1207.821	514.892	1875.608	-57.629
1800	1073.456	2009.414	1279.056	1314.644	517.999	1955.604	-56.749
1900	1082.823	2067.710	1319.042	1422.468	521.105	2035.370	-55.955
2000	1091.068	2123.465	1357.879	1531.172	524.148	2115.002	-55.237
2100	1098.354	2176.878	1395.617	1640.650	527.043	2194.469	-54.583
2200	1104.820	2228.126	1432.301	1750.815	529.787	2273.806	-53.986
2300	1110.579	2277.367	1467.980	1861.591	532.373	2353.019	-53.438
2400	1115.728	2324.743	1502.697	1972.911	534.724	2432.072	-52.932
2500	1120.346	2370.385	1536.498	2084.718	536.852	2511.157	-52.467
2600	1124.502	2414.408	1569.422	2196.964	538.716	2590.032	-52.033
2700	1128.254	2456.919	1601.509	2309.605	540.321	2668.921	-51.632
2800	1131.652	2498.013	1632.798	2422.603	541.638	2747.780	-51.259
2900	1134.737	2537.779	1663.322	2535.925	542.634	2826.538	-50.910
3000	1137.546	2576.296	1693.116	2649.542	543.357	2905.295	-50.585
3100	1140.110	2613.639	1722.211	2763.426	543.722	2983.950	-50.278
3200	1142.457	2649.873	1750.637	2877.556	543.774	3062.679	-49.992
3300	1144.609	2685.062	1778.422	2991.911	543.493	3141.454	-49.724
3400	1146.587	2719.262	1805.593	3106.472	542.848	3220.148	-49.471
3500	1148.410	2752.525	1832.176	3221.223	541.844	3298.846	-49.232
3600	1150.092	2784.901	1858.192	3336.150	540.505	3377.673	-49.008
3700	1151.648	2816.434	1883.667	3451.238	538.797	3456.563	-48.797
3800	1153.090	2847.165	1908.619	3566.475	536.690	3535.436	-48.597
3900	1154.428	2877.135	1933.070	3681.852	534.230	3614.313	-48.407
4000	1155.673	2906.378	1957.039	3797.358	531.397	3693.412	-48.230
4100	1156.832	2934.929	1980.543	3912.984	528.154	3772.503	-48.061
4200	1157.913	2962.819	2003.600	4028.722	524.531	3851.669	-47.902
4300	1158.923	2990.078	2026.225	4144.564	520.512	3930.826	-47.749
4400	1159.868	3016.732	2048.435	4260.504	516.107	4010.183	-47.606
4500	1160.753	3042.807	2070.244	4376.536	511.331	4089.708	-47.471
4600	1161.583	3068.328	2091.665	4492.653	506.128	4169.350	-47.343
4700	1162.363	3093.318	2112.712	4608.851	500.514	4248.984	-47.221
4800	1163.097	3117.798	2133.397	4725.124	494.540	4328.859	-47.107
4900	1163.787	3141.787	2153.732	4841.468	488.125	4408.713	-46.996
5000	1164.438	3165.305	2173.729	4957.880	481.372	4488.910	-46.894

3.481. Benzo[*q*]hexaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-74-5
Point Group: C_s

Length: 18.47 Å
Width: 10.93 Å
Breadth: 3.889 Å
L/B Ratio: 1.689

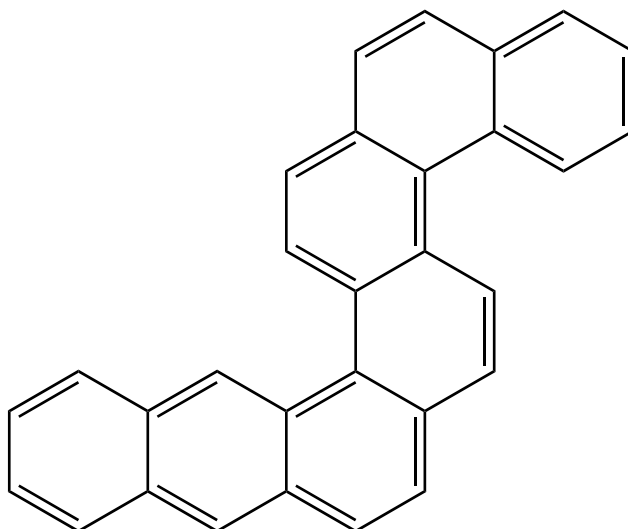
Cartesian coordinates:

C	6.6691	-2.6863	0.0000	C	-1.4191	0.8804	0.0000	H	3.2542	-2.7058	0.0000
C	6.8871	-1.3228	0.0000	C	-1.1536	2.2867	0.0000	H	5.1979	-4.2717	0.0000
C	4.2869	-2.3244	0.0000	C	-2.2636	3.2181	0.0000	H	7.0613	1.3515	0.0000
C	5.3627	-3.1893	0.0000	C	-3.5386	2.7892	0.0000	H	5.1614	2.9449	0.0000
C	4.4878	-0.9324	0.0000	C	-2.8038	0.4180	0.0000	H	2.7677	3.3731	0.0000
C	5.8002	-0.4304	0.0000	C	-3.8595	1.3764	0.0000	H	1.8619	-1.5455	0.0000
C	6.0245	0.9957	0.0000	C	-5.1765	0.9568	0.0000	H	0.3531	3.8230	0.0000
C	4.9909	1.8620	0.0000	C	-3.1090	-0.9302	0.0000	H	-0.5724	-1.0919	0.0000
C	3.3640	-0.0087	0.0000	C	-4.4495	-1.3711	0.0000	H	-2.0278	4.2889	0.0000
C	3.6232	1.3953	0.0000	C	-5.4933	-0.4190	0.0000	H	-4.3737	3.4997	0.0000
C	2.5713	2.2936	0.0000	C	-6.8453	-0.8694	0.0000	H	-5.9909	1.6919	0.0000
C	2.0568	-0.4609	0.0000	C	-7.1264	-2.2060	0.0000	H	-2.2915	-1.6693	0.0000
C	0.9755	0.4455	0.0000	C	-6.0786	-3.1615	0.0000	H	-7.6490	-0.1245	0.0000
C	1.2351	1.8382	0.0000	C	-4.7736	-2.7588	0.0000	H	-8.1633	-2.5576	0.0000
C	0.1455	2.7456	0.0000	H	7.5166	-3.3795	0.0000	H	-6.3334	-4.2264	0.0000
C	-0.3669	-0.0092	0.0000	H	7.9087	-0.9257	0.0000	H	-3.9579	-3.4905	0.0000

Table 3.481: Table of thermodynamic data as a function of temperature for Benzo[*q*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.115	497.409	497.409	∞
100	125.803	380.986	873.977	-49.299	527.052	582.464	-304.242
200	246.608	503.184	658.084	-30.980	511.345	644.142	-168.229
250	316.817	565.700	633.327	-16.907	503.974	678.194	-141.698
298.15	385.273	627.369	627.369	0.000	497.409	712.361	-124.800
300	387.872	629.760	627.376	0.715	497.167	713.693	-124.262
350	456.227	694.736	632.352	21.835	491.116	750.273	-111.970
400	519.670	759.861	644.222	46.255	485.863	787.653	-102.855
450	577.204	824.451	660.667	73.703	481.322	825.654	-95.837
500	628.695	887.982	680.233	103.875	477.396	864.151	-90.275
600	715.204	1010.563	725.164	171.240	471.060	942.132	-82.018
700	783.797	1126.163	774.278	246.319	466.507	1021.034	-76.189
800	838.943	1234.553	825.112	327.552	463.533	1100.461	-71.851
900	883.976	1336.052	876.306	413.772	461.937	1180.170	-68.494
1000	921.241	1431.177	927.088	504.089	461.528	1260.005	-65.815
1100	952.400	1520.485	977.016	597.817	462.085	1339.844	-63.623
1200	978.671	1604.513	1025.841	694.407	463.443	1419.575	-61.791
1300	1000.977	1683.753	1073.431	793.419	465.396	1499.180	-60.237
1400	1020.032	1758.649	1119.725	894.494	467.795	1578.622	-58.898
1500	1036.403	1829.596	1164.706	997.336	470.545	1657.882	-57.731
1600	1050.540	1896.946	1208.384	1101.700	473.500	1736.940	-56.704
1700	1062.811	1961.012	1250.787	1207.382	476.576	1815.782	-55.791
1800	1073.512	2022.070	1291.954	1314.210	479.688	1894.513	-54.976
1900	1082.888	2080.369	1331.927	1422.040	482.800	1973.013	-54.241
2000	1091.138	2136.128	1370.753	1530.750	485.850	2051.379	-53.575
2100	1098.427	2189.545	1408.480	1640.236	488.752	2129.579	-52.969
2200	1104.895	2240.796	1445.156	1750.408	491.503	2207.649	-52.415
2300	1110.654	2290.040	1480.826	1861.191	494.097	2285.596	-51.906
2400	1115.802	2337.419	1515.537	1972.519	496.456	2363.381	-51.437
2500	1120.419	2383.064	1549.330	2084.334	498.591	2441.198	-51.005
2600	1124.574	2427.090	1582.249	2196.587	500.462	2518.806	-50.602
2700	1128.325	2469.603	1614.331	2309.235	502.074	2596.426	-50.230
2800	1131.720	2510.700	1645.614	2422.240	503.398	2674.017	-49.883
2900	1134.803	2550.468	1676.134	2535.569	504.401	2751.505	-49.559
3000	1137.610	2588.988	1705.924	2649.192	505.131	2828.994	-49.256
3100	1140.172	2626.332	1735.015	2763.083	505.502	2906.379	-48.971
3200	1142.516	2662.569	1763.438	2877.219	505.560	2983.838	-48.705
3300	1144.666	2697.760	1791.220	2991.580	505.285	3061.344	-48.456
3400	1146.643	2731.961	1818.389	3106.146	504.645	3138.768	-48.220
3500	1148.463	2765.226	1844.968	3220.903	503.647	3216.196	-47.998
3600	1150.144	2797.603	1870.982	3335.834	502.313	3293.753	-47.790
3700	1151.698	2829.137	1896.454	3450.927	500.611	3371.373	-47.594
3800	1153.138	2859.870	1921.405	3566.170	498.508	3448.975	-47.408
3900	1154.474	2889.841	1945.854	3681.552	496.053	3526.582	-47.232
4000	1155.717	2919.086	1969.820	3797.062	493.225	3604.410	-47.068
4100	1156.874	2947.638	1993.323	3912.692	489.986	3682.230	-46.911
4200	1157.954	2975.529	2016.378	4028.434	486.367	3760.125	-46.763
4300	1158.962	3002.788	2039.002	4144.281	482.352	3838.011	-46.622
4400	1159.906	3029.443	2061.210	4260.224	477.951	3916.098	-46.489
4500	1160.790	3055.519	2083.017	4376.260	473.179	3994.351	-46.364
4600	1161.619	3081.041	2104.437	4492.381	467.980	4072.722	-46.246
4700	1162.397	3106.032	2125.482	4608.582	462.369	4151.085	-46.133
4800	1163.130	3130.512	2146.166	4724.859	456.399	4229.688	-46.027
4900	1163.819	3154.502	2166.501	4841.206	449.986	4308.271	-45.926
5000	1164.469	3178.021	2186.497	4957.621	443.236	4387.196	-45.832

3.482. Benzo[*c*]naphtho[2,3-*l*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-44-9
Point Group: C₁

Length: 18.12 Å
Width: 10.55 Å
Breadth: 4.852 Å
L/B Ratio: 1.718

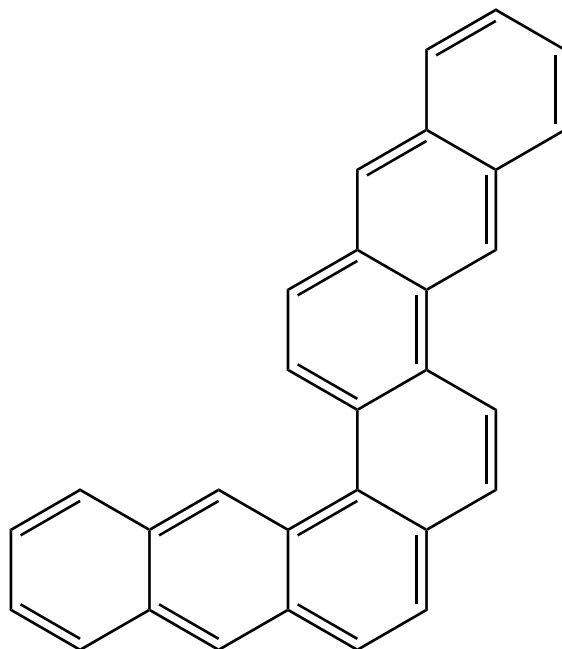
Cartesian coordinates:

C	5.9007	2.5866	0.3485	C	-0.2479	-0.0577	-0.1380	H	7.1426	-0.4962	-0.4632
C	6.8403	1.5729	0.0166	C	-1.5798	-0.4726	0.0948	H	3.8410	3.0741	0.6912
C	6.4268	0.2941	-0.2106	C	-1.0351	2.2053	-0.5301	H	5.3118	-2.1553	-0.4869
C	4.5714	2.2979	0.4359	C	-0.0321	1.2902	-0.5547	H	2.0380	1.4652	0.5135
C	4.1033	0.9699	0.1919	C	-2.3640	1.8132	-0.2068	H	3.5756	-3.8042	-0.4229
C	5.0413	-0.0409	-0.1207	C	-2.6771	0.4579	-0.0474	H	1.2153	-4.4077	0.0818
C	4.5844	-1.3553	-0.2998	C	-4.6508	2.4987	0.1730	H	-0.9812	-3.7772	0.7595
C	2.7347	0.6566	0.2490	C	-3.3592	2.8312	-0.0640	H	-2.7922	-2.1241	0.8561
C	2.2615	-0.6250	-0.0091	C	-5.0475	1.1241	0.1447	H	-0.8427	3.2537	-0.7871
C	3.2310	-1.6555	-0.2114	C	-4.0857	0.1061	-0.0351	H	0.9669	1.5988	-0.8912
C	2.8174	-3.0349	-0.2371	C	-4.5737	-1.2004	-0.2805	H	-5.4144	3.2662	0.3430
C	1.5344	-3.3608	0.0208	C	-5.9161	-1.4914	-0.2322	H	-3.0467	3.8801	-0.1247
C	0.8452	-0.9840	0.0062	C	-6.8530	-0.4858	0.0589	H	-3.8697	-2.0036	-0.5360
C	0.5357	-2.3368	0.1764	C	-6.4234	0.8068	0.2299	H	-6.2648	-2.5110	-0.4271
C	-0.7870	-2.7295	0.5010	H	6.2649	3.6028	0.5318	H	-7.9164	-0.7365	0.1260
C	-1.7945	-1.8132	0.5188	H	7.9004	1.8383	-0.0507	H	-7.1432	1.6116	0.4190

Table 3.482: Table of thermodynamic data as a function of temperature for Benzo[*c*]naphtho[2,3-*l*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.733	546.708	546.708	∞
100	123.949	373.006	864.271	-49.126	576.523	632.733	-330.499
200	245.775	494.234	648.941	-30.941	560.682	695.269	-181.582
250	316.436	556.613	624.207	-16.898	553.281	729.773	-152.475
298.15	385.298	618.251	618.251	0.000	546.708	764.378	-133.913
300	387.911	620.642	618.258	0.715	546.466	765.727	-133.322
350	456.633	685.652	623.235	21.846	540.426	802.762	-119.803
400	520.361	750.851	635.114	46.295	535.201	840.594	-109.768
450	578.090	815.534	651.575	73.782	530.699	879.044	-102.035
500	629.693	879.165	671.163	104.001	526.821	917.985	-95.899
600	716.244	1001.936	716.152	171.470	520.588	996.837	-86.781
700	784.739	1117.689	765.333	246.649	516.135	1076.594	-80.335
800	839.736	1226.195	816.234	327.969	513.249	1156.862	-75.534
900	884.615	1327.779	867.491	414.260	511.724	1237.402	-71.815
1000	921.742	1422.964	918.330	504.635	511.372	1318.062	-68.847
1100	952.786	1512.315	968.309	598.406	511.973	1398.719	-66.418
1200	978.964	1596.372	1017.180	695.030	513.364	1479.266	-64.389
1300	1001.197	1675.632	1064.811	794.068	515.343	1559.685	-62.668
1400	1020.195	1750.542	1111.141	895.162	517.761	1639.938	-61.186
1500	1036.521	1821.499	1156.154	998.018	520.525	1720.007	-59.895
1600	1050.624	1888.856	1199.861	1102.392	523.490	1799.875	-58.759
1700	1062.869	1952.925	1242.290	1208.081	526.573	1879.526	-57.750
1800	1073.550	2013.987	1283.479	1314.913	529.690	1959.065	-56.849
1900	1082.910	2072.287	1323.473	1422.747	532.805	2038.373	-56.038
2000	1091.148	2128.047	1362.318	1531.458	535.857	2117.547	-55.304
2100	1098.429	2181.464	1400.062	1640.944	538.759	2196.556	-54.635
2200	1104.889	2232.715	1436.753	1751.117	541.510	2275.434	-54.025
2300	1110.644	2281.958	1472.437	1861.899	544.103	2354.189	-53.464
2400	1115.788	2329.338	1507.160	1973.225	546.460	2432.782	-52.947
2500	1120.402	2374.981	1540.966	2085.039	548.594	2511.408	-52.472
2600	1124.555	2419.007	1573.895	2197.290	550.464	2589.824	-52.029
2700	1128.304	2461.519	1605.987	2309.936	552.074	2668.252	-51.619
2800	1131.698	2502.615	1637.280	2422.939	553.395	2746.651	-51.238
2900	1134.781	2542.383	1667.809	2536.265	554.396	2824.949	-50.882
3000	1137.587	2580.902	1697.606	2649.886	555.123	2903.245	-50.549
3100	1140.149	2618.245	1726.705	2763.774	555.492	2981.440	-50.236
3200	1142.493	2654.481	1755.135	2877.908	555.548	3059.708	-49.944
3300	1144.643	2689.671	1782.923	2992.267	555.270	3138.022	-49.670
3400	1146.620	2723.872	1810.098	3106.831	554.629	3216.255	-49.411
3500	1148.441	2757.136	1836.683	3221.585	553.628	3294.492	-49.167
3600	1150.122	2789.512	1862.703	3336.515	552.292	3372.858	-48.938
3700	1151.676	2821.046	1888.180	3451.606	550.587	3451.287	-48.722
3800	1153.117	2851.779	1913.135	3566.846	548.483	3529.698	-48.518
3900	1154.454	2881.749	1937.589	3682.226	546.025	3608.114	-48.324
4000	1155.697	2910.993	1961.560	3797.734	543.195	3686.751	-48.143
4100	1156.855	2939.545	1985.066	3913.362	539.955	3765.381	-47.971
4200	1157.935	2967.435	2008.125	4029.102	536.334	3844.086	-47.807
4300	1158.944	2994.694	2030.753	4144.947	532.316	3922.781	-47.651
4400	1159.888	3021.348	2052.964	4260.889	527.913	4001.677	-47.505
4500	1160.772	3047.424	2074.775	4376.922	523.140	4080.740	-47.367
4600	1161.602	3072.946	2096.198	4493.042	517.939	4159.920	-47.236
4700	1162.381	3097.936	2117.246	4609.241	512.327	4239.093	-47.111
4800	1163.114	3122.416	2137.933	4725.516	506.355	4318.505	-46.994
4900	1163.804	3146.406	2158.270	4841.862	499.941	4397.898	-46.881
5000	1164.454	3169.924	2178.269	4958.276	493.189	4477.633	-46.777

3.483. Benzo[*b*]naphtho[2,3-*l*]chrysene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-71-2
Point Group: C_1

Length: 18.58 Å
Width: 10.73 Å
Breadth: 5.215 Å
L/B Ratio: 1.732

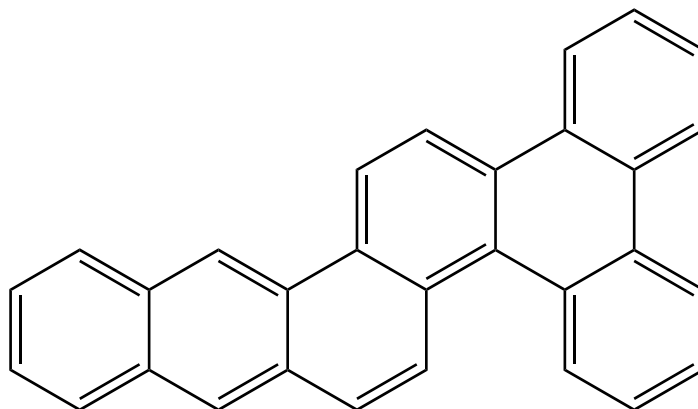
Cartesian coordinates:

C	-5.5374	3.1463	0.5123	C	0.0675	-0.4290	-0.2415	H	-7.2998	0.3042	-0.2080
C	-6.6440	2.2965	0.2433	C	1.3062	-1.0515	-0.0156	H	-3.4093	3.2986	0.7275
C	-6.4533	0.9691	-0.0030	C	1.2230	1.6548	-0.8020	H	-5.7607	-1.6223	-0.3497
C	-4.2676	2.6493	0.5207	C	0.0827	0.9393	-0.6990	H	-1.8971	1.4229	0.4483
C	-4.0327	1.2652	0.2564	C	2.4941	1.0829	-0.4453	H	-4.3078	-3.5252	-0.4073
C	-5.1360	0.4183	0.0041	C	2.5415	-0.2857	-0.0630	H	-2.0483	-4.5071	-0.0843
C	-4.9051	-0.9511	-0.2030	C	3.7679	-0.8536	0.2604	H	0.2680	-4.2830	0.3230
C	-2.7298	0.7369	0.2354	C	3.6559	1.8422	-0.4859	H	2.3389	-2.9077	0.4304
C	-2.4845	-0.6025	-0.0405	C	4.8938	1.2692	-0.1515	H	1.2074	2.6875	-1.1698
C	-3.6148	-1.4630	-0.1950	C	4.9493	-0.0950	0.2241	H	-0.8691	1.3985	-0.9999
C	-3.4261	-2.8902	-0.2634	C	6.2127	-0.6717	0.5605	H	3.8140	-1.9156	0.5498
C	-2.1979	-3.4211	-0.1020	C	7.3473	0.0824	0.5204	H	3.6120	2.8980	-0.7806
C	-1.1431	-1.1799	-0.0941	C	7.2911	1.4520	0.1440	H	6.2469	-1.7281	0.8497
C	-1.0368	-2.5756	0.0120	C	6.1017	2.0317	-0.1829	H	8.3180	-0.3543	0.7770
C	0.2203	-3.1948	0.1985	H	-5.7231	4.2067	0.7121	H	8.2200	2.0312	0.1217
C	1.3610	-2.4415	0.2363	H	-7.6509	2.7266	0.2395	H	6.0484	3.0867	-0.4743

Table 3.483: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[2,3-*l*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.993	522.575	522.575	∞
100	124.926	374.565	867.890	-49.332	552.185	608.238	-317.705
200	246.822	496.511	651.729	-31.044	536.447	670.579	-175.134
250	317.485	559.124	626.917	-16.948	529.099	704.963	-147.291
298.15	386.307	620.944	620.944	0.000	522.575	739.442	-129.545
300	388.918	623.341	620.951	0.717	522.335	740.786	-128.980
350	457.551	688.500	625.940	21.896	516.343	777.683	-116.060
400	521.168	753.814	637.845	46.388	511.162	815.370	-106.474
450	578.788	818.586	654.336	73.912	506.698	853.669	-99.089
500	630.295	882.286	673.957	104.164	502.852	892.455	-93.232
600	716.707	1005.152	719.010	171.686	496.672	970.990	-84.530
700	785.124	1120.971	768.247	246.907	492.261	1050.422	-78.382
800	840.079	1229.526	819.196	328.263	489.410	1130.360	-73.803
900	884.935	1331.148	870.496	414.587	487.918	1210.565	-70.258
1000	922.046	1426.366	921.373	504.993	487.598	1290.886	-67.428
1100	953.077	1515.745	971.387	598.794	488.228	1371.202	-65.112
1200	979.243	1599.827	1020.288	695.446	489.649	1451.404	-63.177
1300	1001.463	1679.109	1067.947	794.511	491.654	1531.476	-61.534
1400	1020.447	1754.038	1114.302	895.631	494.098	1611.380	-60.120
1500	1036.760	1825.012	1159.338	998.512	496.887	1691.100	-58.888
1600	1050.850	1892.384	1203.066	1102.909	499.875	1770.615	-57.803
1700	1063.081	1956.467	1245.514	1208.620	502.980	1849.912	-56.840
1800	1073.750	2017.540	1286.721	1315.474	506.118	1929.097	-55.980
1900	1083.098	2075.850	1326.731	1423.326	509.252	2008.049	-55.204
2000	1091.325	2131.620	1365.592	1532.056	512.322	2086.867	-54.502
2100	1098.595	2185.045	1403.350	1641.559	515.241	2165.518	-53.863
2200	1105.045	2236.304	1440.055	1751.747	518.009	2244.037	-53.279
2300	1110.791	2285.554	1475.752	1862.545	520.617	2322.433	-52.743
2400	1115.926	2332.939	1510.487	1973.885	522.988	2400.666	-52.248
2500	1120.532	2378.589	1544.304	2085.712	525.135	2478.931	-51.793
2600	1124.677	2422.619	1577.243	2197.976	527.017	2556.986	-51.369
2700	1128.419	2465.136	1609.345	2310.634	528.639	2635.053	-50.977
2800	1131.807	2506.236	1640.647	2423.648	529.973	2713.090	-50.612
2900	1134.884	2546.007	1671.185	2536.985	530.984	2791.025	-50.271
3000	1137.685	2584.529	1700.991	2650.616	531.721	2868.960	-49.952
3100	1140.242	2621.876	1730.097	2764.514	532.099	2946.791	-49.652
3200	1142.581	2658.115	1758.535	2878.657	532.164	3024.696	-49.372
3300	1144.727	2693.307	1786.330	2993.024	531.895	3102.647	-49.110
3400	1146.699	2727.511	1813.512	3107.597	531.262	3180.516	-48.862
3500	1148.517	2760.777	1840.103	3222.359	530.269	3258.389	-48.628
3600	1150.194	2793.156	1866.129	3337.295	528.941	3336.391	-48.409
3700	1151.745	2824.691	1891.612	3452.393	527.242	3414.455	-48.202
3800	1153.182	2855.426	1916.573	3567.641	525.145	3492.502	-48.007
3900	1154.516	2885.398	1941.032	3683.026	522.693	3570.553	-47.821
4000	1155.757	2914.643	1965.008	3798.541	519.870	3648.825	-47.648
4100	1156.912	2943.196	1988.519	3914.175	516.635	3727.090	-47.483
4200	1157.990	2971.088	2011.583	4029.921	513.020	3805.429	-47.326
4300	1158.997	2998.348	2034.215	4145.770	509.008	3883.759	-47.177
4400	1159.938	3025.004	2056.431	4261.718	504.610	3962.290	-47.037
4500	1160.821	3051.081	2078.246	4377.756	499.841	4040.987	-46.906
4600	1161.648	3076.604	2099.673	4493.880	494.645	4119.802	-46.781
4700	1162.426	3101.595	2120.726	4610.084	489.037	4198.608	-46.661
4800	1163.157	3126.075	2141.416	4726.364	483.070	4277.655	-46.549
4900	1163.845	3150.066	2161.757	4842.714	476.660	4356.681	-46.442
5000	1164.494	3173.585	2181.759	4959.131	469.912	4436.051	-46.342

3.484. Dibenzo[*b,j*]plcene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-48-3
Point Group: C₁

Length: 18.00 Å
Width: 10.86 Å
Breadth: 5.175 Å
L/B Ratio: 1.657

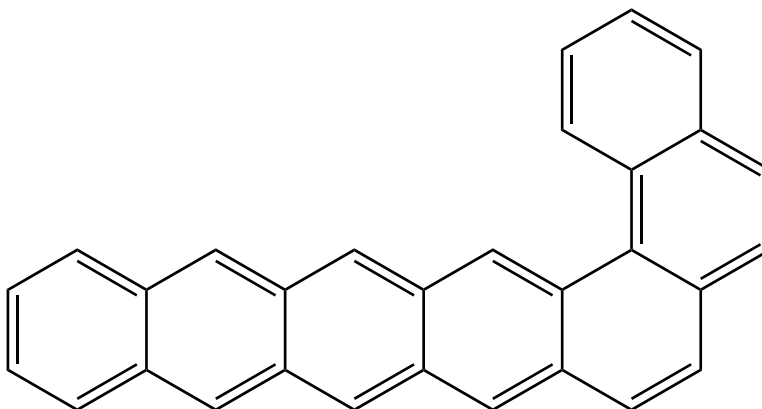
Cartesian coordinates:

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C	-7.4013	0.1003	-0.0060	C	1.4312	-0.2413	-0.0575	H	-5.3767	2.7552	-0.7501
C	-6.4643	-0.8484	0.2767	C	3.1971	1.5069	-0.0019	H	-4.3901	-2.5067	0.7809
C	-5.6886	1.7450	-0.4622	C	4.1914	0.5265	0.1326	H	-3.0113	2.1130	-0.5394
C	-4.6808	0.7743	-0.1728	C	5.5238	0.9195	0.3596	H	-2.0409	-3.1234	1.0678
C	-5.0727	-0.5343	0.2003	C	5.8650	2.2544	0.4267	H	0.3400	-2.6024	0.8189
C	-4.0877	-1.4937	0.4880	C	4.8804	3.2344	0.2594	H	1.1293	3.1551	-0.4025
C	-3.3153	1.0937	-0.2522	C	3.5680	2.8648	0.0487	H	-1.2809	2.5514	-0.4803
C	-2.3408	0.1433	0.0257	C	3.8337	-0.8717	-0.0249	H	6.2939	0.1415	0.4735
C	-2.7409	-1.1674	0.4041	C	2.4845	-1.2458	-0.1811	H	6.9037	2.5507	0.6052
C	-1.7225	-2.1375	0.7090	C	2.2158	-2.5805	-0.5427	H	5.1547	4.2935	0.3005
C	-0.4127	-1.8430	0.5659	C	3.2201	-3.5224	-0.6415	H	2.7925	3.6353	-0.0763
C	-0.9229	0.4527	-0.0629	C	4.5458	-3.1621	-0.3871	H	1.1829	-2.8878	-0.7564
C	0.0443	-0.5491	0.1190	C	4.8449	-1.8481	-0.0950	H	2.9802	-4.5532	-0.9227
C	0.8150	2.1065	-0.2890	H	-7.7848	2.1538	-0.6009	H	5.3389	-3.9149	-0.4381
C	-0.5136	1.7810	-0.3093	H	-8.4693	-0.1344	0.0507	H	5.8886	-1.5419	0.0751

Table 3.484: Table of thermodynamic data as a function of temperature for Dibenzob[*b,j*]plcene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.116	519.259	519.259	∞
100	126.400	375.937	869.462	-49.353	548.848	604.765	-315.890
200	246.816	498.473	653.409	-30.987	533.187	666.926	-174.180
250	316.859	561.014	628.648	-16.908	525.822	701.214	-146.508
298.15	385.322	622.689	622.689	0.000	519.259	735.605	-128.872
300	387.924	625.081	622.697	0.715	519.017	736.946	-128.311
350	456.396	690.073	627.673	21.840	512.970	773.760	-115.475
400	519.982	755.229	639.548	46.273	507.730	811.372	-105.952
450	577.637	819.863	655.999	73.739	503.207	849.604	-98.617
500	629.205	883.445	675.575	103.935	499.305	888.329	-92.801
600	715.747	1006.124	720.535	171.354	493.023	966.758	-84.162
700	784.262	1121.802	769.683	246.484	488.521	1046.101	-78.059
800	839.287	1230.247	820.550	327.758	485.588	1125.960	-73.516
900	884.195	1331.780	871.774	414.005	484.020	1206.098	-69.999
1000	921.350	1426.922	922.583	504.339	483.628	1286.360	-67.191
1100	952.421	1516.236	972.533	598.073	484.190	1366.624	-64.894
1200	978.625	1600.262	1021.378	694.661	485.547	1446.780	-62.975
1300	1000.883	1679.497	1068.984	793.666	487.493	1526.811	-61.347
1400	1019.904	1754.384	1115.291	894.730	489.881	1606.678	-59.945
1500	1036.252	1825.322	1160.283	997.558	492.617	1686.365	-58.723
1600	1050.375	1892.662	1203.970	1101.906	495.556	1765.851	-57.648
1700	1062.638	1956.717	1246.381	1207.571	498.615	1845.122	-56.693
1800	1073.336	2017.765	1287.553	1314.382	501.709	1924.283	-55.840
1900	1082.711	2076.054	1327.531	1422.194	504.804	2003.214	-55.071
2000	1090.963	2131.804	1366.361	1530.887	507.836	2082.012	-54.375
2100	1098.257	2185.213	1404.091	1640.355	510.721	2160.645	-53.742
2200	1104.729	2236.456	1440.769	1750.511	513.455	2239.149	-53.163
2300	1110.494	2285.693	1476.442	1861.277	516.033	2317.529	-52.632
2400	1115.648	2333.066	1511.154	1972.589	518.376	2395.750	-52.141
2500	1120.271	2378.704	1544.948	2084.389	520.496	2474.003	-51.690
2600	1124.432	2422.725	1577.868	2196.628	522.353	2552.046	-51.270
2700	1128.188	2465.233	1609.950	2309.262	523.951	2630.103	-50.881
2800	1131.590	2506.325	1641.234	2422.254	525.261	2708.131	-50.520
2900	1134.678	2546.088	1671.754	2535.570	526.251	2786.058	-50.181
3000	1137.491	2584.604	1701.544	2649.180	526.969	2863.985	-49.865
3100	1140.058	2621.944	1730.635	2763.060	527.328	2941.809	-49.568
3200	1142.407	2658.177	1759.057	2877.185	527.375	3019.707	-49.291
3300	1144.562	2693.365	1786.839	2991.535	527.089	3097.652	-49.031
3400	1146.543	2727.563	1814.007	3106.091	526.440	3175.516	-48.785
3500	1148.367	2760.825	1840.586	3220.838	525.431	3253.384	-48.553
3600	1150.052	2793.200	1866.600	3335.760	524.089	3331.381	-48.336
3700	1151.610	2824.731	1892.071	3450.844	522.377	3409.441	-48.132
3800	1153.053	2855.462	1917.021	3566.078	520.266	3487.484	-47.938
3900	1154.393	2885.431	1941.469	3681.451	517.802	3565.532	-47.754
4000	1155.639	2914.673	1965.435	3796.954	514.966	3643.801	-47.582
4100	1156.800	2943.224	1988.937	3912.576	511.720	3722.063	-47.419
4200	1157.882	2971.113	2011.991	4028.311	508.094	3800.399	-47.264
4300	1158.894	2998.370	2034.614	4144.150	504.071	3878.727	-47.116
4400	1159.840	3025.024	2056.822	4260.088	499.663	3957.255	-46.978
4500	1160.726	3051.099	2078.628	4376.116	494.885	4035.950	-46.847
4600	1161.557	3076.619	2100.047	4492.231	489.680	4114.763	-46.724
4700	1162.338	3101.608	2121.092	4608.426	484.063	4193.569	-46.605
4800	1163.073	3126.087	2141.776	4724.697	478.087	4272.614	-46.495
4900	1163.764	3150.076	2162.109	4841.039	471.669	4351.639	-46.388
5000	1164.416	3173.594	2182.104	4957.449	464.913	4431.008	-46.289

3.485. Naphtho[1,2-*a*]pentacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115791-74-7
Point Group: C₁

Length: 18.36 Å
Width: 10.61 Å
Breadth: 4.893 Å
L/B Ratio: 1.730

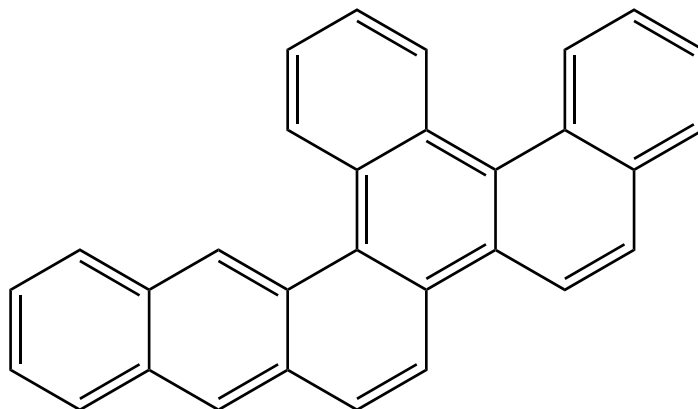
Cartesian coordinates:

C	3.1389	2.0772	0.6102	C	-0.3994	-0.1991	-0.0979	H	-7.0894	-1.8586	0.4253
C	3.9117	0.9960	0.1089	C	0.9729	0.1807	-0.1799	H	-5.9431	2.9060	-0.5983
C	5.2642	1.2638	-0.2014	C	-2.0626	-1.9425	0.2924	H	-4.6998	-2.4233	0.4737
C	5.7708	2.5869	-0.1269	C	-3.0921	-1.0023	0.1326	H	-3.5537	2.3423	-0.5476
C	4.9763	3.6132	0.3098	C	-2.7653	0.3559	-0.1564	H	-2.3136	-2.9883	0.5087
C	3.6513	3.3448	0.7070	C	-1.4188	0.7360	-0.2676	H	-1.1705	1.7818	-0.4874
C	6.1463	0.2006	-0.5475	C	-4.4541	-1.3778	0.2498	H	0.0822	-3.5583	0.4383
C	5.7058	-1.0854	-0.5033	C	-5.4592	-0.4471	0.0854	H	1.1853	1.2363	-0.4046
C	4.3414	-1.3723	-0.2147	C	-5.1309	0.9178	-0.2075	H	2.4022	-4.1557	0.3160
C	3.4121	-0.3504	-0.0268	C	-3.8101	1.2994	-0.3235	H	4.7490	-3.5177	-0.1800
C	3.9616	-2.7597	-0.0934	C	-6.8484	-0.8132	0.2011	H	6.3895	-1.9184	-0.7052
C	2.6869	-3.1086	0.1613	C	-7.8238	0.1119	0.0363	H	7.1835	0.4343	-0.8133
C	1.6456	-2.1074	0.1864	C	-7.4958	1.4755	-0.2567	H	6.8129	2.7706	-0.4131
C	1.9953	-0.7163	0.0152	C	-6.2040	1.8654	-0.3743	H	5.3620	4.6359	0.3702
C	0.3344	-2.5004	0.2908	H	-8.3142	2.1918	-0.3826	H	3.0356	4.1604	1.1007
C	-0.7283	-1.5594	0.1762	H	-8.8804	-0.1617	0.1231	H	2.1091	1.8944	0.9465

Table 3.485: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*a*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-57.286	556.172	556.172	∞
100	125.566	379.572	874.722	-49.515	585.599	641.152	-334.896
200	247.751	502.004	657.775	-31.154	569.934	702.966	-183.592
250	318.630	564.850	632.875	-17.006	562.637	737.070	-153.999
298.15	387.566	626.882	626.882	0.000	556.172	771.268	-135.120
300	390.180	629.287	626.889	0.719	555.934	772.602	-134.519
350	458.842	694.644	631.894	21.963	550.006	809.196	-120.763
400	522.431	760.129	643.833	46.518	544.889	846.571	-110.549
450	579.993	825.047	660.370	74.105	540.486	884.551	-102.674
500	631.429	888.870	680.039	104.415	536.699	923.011	-96.424
600	717.696	1011.930	725.192	172.043	530.625	1000.877	-87.132
700	785.984	1127.891	774.525	247.356	526.307	1079.624	-80.561
800	840.833	1236.553	825.562	328.793	523.537	1158.863	-75.664
900	885.602	1338.260	876.940	415.188	522.115	1238.361	-71.871
1000	922.641	1433.544	927.888	505.656	521.858	1317.968	-68.842
1100	953.610	1522.976	977.964	599.514	522.545	1397.563	-66.363
1200	979.723	1607.103	1026.922	696.217	524.016	1477.041	-64.293
1300	1001.897	1686.422	1074.631	795.328	526.067	1556.383	-62.535
1400	1020.842	1761.381	1121.032	896.489	528.553	1635.554	-61.022
1500	1037.119	1832.381	1166.110	999.407	531.379	1714.538	-59.704
1600	1051.178	1899.775	1209.876	1103.839	534.401	1793.315	-58.545
1700	1063.381	1963.877	1252.359	1209.581	537.538	1871.873	-57.514
1800	1074.025	2024.966	1293.598	1316.463	540.704	1950.316	-56.596
1900	1083.351	2083.291	1333.638	1424.342	543.865	2028.524	-55.767
2000	1091.559	2139.073	1372.525	1533.096	546.959	2106.597	-55.018
2100	1098.811	2192.509	1410.308	1642.622	549.901	2184.502	-54.335
2200	1105.246	2243.778	1447.036	1752.831	552.689	2262.275	-53.712
2300	1110.977	2293.037	1482.755	1863.648	555.316	2339.922	-53.140
2400	1116.099	2340.429	1517.510	1975.006	557.706	2417.407	-52.612
2500	1120.694	2386.086	1551.346	2086.850	559.870	2494.923	-52.127
2600	1124.828	2430.122	1584.303	2199.130	561.767	2572.228	-51.676
2700	1128.561	2472.645	1616.422	2311.802	563.404	2649.544	-51.257
2800	1131.940	2513.750	1647.739	2424.830	564.751	2726.830	-50.869
2900	1135.009	2553.525	1678.291	2538.180	565.775	2804.014	-50.505
3000	1137.802	2592.052	1708.111	2651.823	566.524	2881.196	-50.165
3100	1140.352	2629.402	1737.231	2765.732	566.914	2958.274	-49.846
3200	1142.686	2665.644	1765.680	2879.886	566.990	3035.426	-49.547
3300	1144.826	2700.840	1793.488	2994.263	566.731	3112.624	-49.268
3400	1146.793	2735.046	1820.680	3108.845	566.107	3189.740	-49.003
3500	1148.605	2768.315	1847.282	3223.616	565.123	3266.860	-48.754
3600	1150.278	2800.696	1873.318	3338.562	563.803	3344.108	-48.521
3700	1151.825	2832.234	1898.810	3453.668	562.114	3421.418	-48.301
3800	1153.259	2862.971	1923.780	3568.923	560.024	3498.710	-48.092
3900	1154.589	2892.944	1948.248	3684.316	557.580	3576.007	-47.894
4000	1155.826	2922.192	1972.232	3799.838	554.763	3653.524	-47.709
4100	1156.978	2950.747	1995.752	3915.479	551.535	3731.034	-47.533
4200	1158.053	2978.640	2018.823	4031.231	547.926	3808.618	-47.366
4300	1159.057	3005.901	2041.463	4147.087	543.921	3886.193	-47.207
4400	1159.996	3032.558	2063.686	4263.040	539.529	3963.968	-47.057
4500	1160.876	3058.637	2085.507	4379.084	534.766	4041.909	-46.916
4600	1161.701	3084.161	2106.940	4495.213	529.575	4119.968	-46.783
4700	1162.477	3109.153	2127.999	4611.423	523.972	4198.019	-46.655
4800	1163.206	3133.635	2148.696	4727.707	518.010	4276.310	-46.535
4900	1163.892	3157.626	2169.042	4844.062	511.605	4354.580	-46.419
5000	1164.539	3181.147	2189.050	4960.484	504.862	4433.194	-46.312

3.486. Dibenzo[*b,s*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-88-1
Point Group: C₁

Length: 18.20 Å
Width: 10.47 Å
Breadth: 4.976 Å
L/B Ratio: 1.738

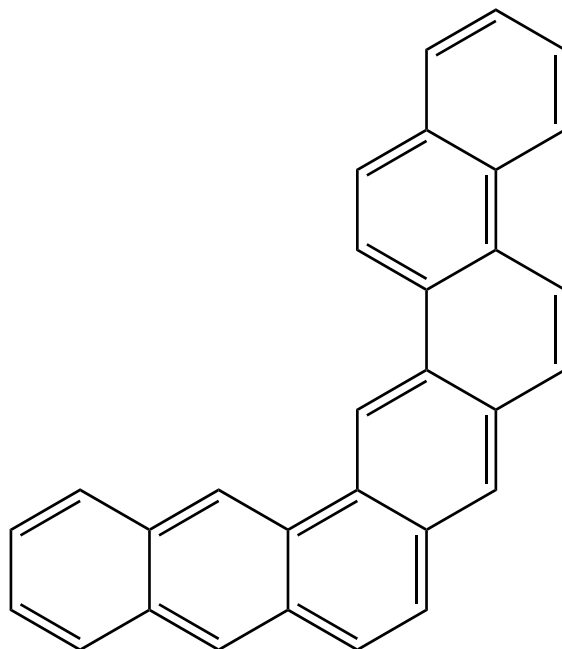
Cartesian coordinates:

C	6.4589	1.3065	-0.5564	C	-2.1002	2.4997	-0.2785	H	6.5528	-1.9685	0.4312
C	6.9883	0.0404	-0.1811	C	-1.3645	3.6418	-0.0741	H	4.6978	2.4857	-0.8759
C	6.1566	-0.9880	0.1442	C	-0.0534	3.5377	0.4110	H	4.2501	-2.8494	0.6231
C	5.1128	1.5131	-0.5879	C	0.5237	2.2970	0.5322	H	2.4511	1.6493	-0.5416
C	4.2106	0.4585	-0.2411	C	-2.3922	0.0208	-0.0629	H	2.0231	-3.7513	0.7263
C	4.7390	-0.8053	0.1149	C	-1.7454	-1.2153	-0.0943	H	-0.4009	-3.4873	0.3340
C	3.8524	-1.8523	0.3960	C	-2.4912	-2.4050	-0.3698	H	-3.1308	2.5960	-0.6464
C	2.8223	0.6582	-0.2428	C	-3.8342	-2.3692	-0.5534	H	-1.7990	4.6273	-0.2695
C	1.9303	-0.3519	0.1116	C	-3.8413	0.0306	-0.0295	H	0.5067	4.4413	0.6723
C	2.4767	-1.6461	0.3622	C	-4.5463	-1.1519	-0.3399	H	1.5586	2.2300	0.8950
C	1.5929	-2.7686	0.5014	C	-5.9617	-1.1621	-0.3806	H	-1.9506	-3.3588	-0.4588
C	0.2662	-2.6132	0.3044	C	-6.6751	-0.0406	-0.0434	H	-4.3933	-3.2716	-0.8259
C	0.4824	-0.1783	0.1514	C	-5.9887	1.1146	0.3722	H	-6.4770	-2.0846	-0.6723
C	-0.3166	-1.3140	0.1000	C	-4.6161	1.1451	0.3814	H	-7.7692	-0.0405	-0.0740
C	-0.1765	1.1105	0.2067	H	7.1542	2.1107	-0.8186	H	-6.5605	1.9912	0.6948
C	-1.5667	1.2115	-0.0344	H	8.0752	-0.0907	-0.1608	H	-4.1134	2.0554	0.7346

Table 3.486: Table of thermodynamic data as a function of temperature for Dibenzo[*b,s*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.847	560.915	560.915	∞
100	125.102	371.617	864.038	-49.242	590.615	646.964	-337.932
200	246.287	493.536	648.344	-30.962	574.870	709.596	-185.324
250	316.607	555.989	623.598	-16.902	567.485	744.133	-155.475
298.15	385.310	617.641	617.641	0.000	560.915	778.767	-136.434
300	387.920	620.033	617.649	0.715	560.674	780.117	-135.828
350	456.589	685.039	622.626	21.845	554.632	817.183	-121.955
400	520.316	750.232	634.504	46.291	549.406	855.047	-111.655
450	578.061	814.911	650.963	73.776	544.902	893.527	-103.716
500	629.680	878.540	670.550	103.995	541.022	932.499	-97.415
600	716.246	1001.309	715.537	171.463	534.790	1011.414	-88.050
700	784.730	1117.062	764.717	246.642	530.336	1091.234	-81.427
800	839.704	1225.566	815.616	327.960	527.448	1171.564	-76.494
900	884.558	1327.145	866.871	414.246	525.918	1252.168	-72.672
1000	921.663	1422.322	917.708	504.614	525.560	1332.891	-69.622
1100	952.690	1511.664	967.685	598.377	526.151	1413.614	-67.126
1200	978.857	1595.713	1016.554	694.991	527.533	1494.226	-65.041
1300	1001.083	1674.964	1064.182	794.017	529.501	1574.711	-63.271
1400	1020.079	1749.866	1110.509	895.100	531.907	1655.031	-61.749
1500	1036.404	1820.815	1155.519	997.944	534.660	1735.169	-60.423
1600	1050.509	1888.164	1199.222	1102.307	537.613	1815.105	-59.256
1700	1062.757	1952.227	1241.648	1207.984	540.685	1894.825	-58.220
1800	1073.442	2013.281	1282.834	1314.806	543.790	1974.435	-57.295
1900	1082.806	2071.576	1322.824	1422.628	546.895	2053.814	-56.462
2000	1091.048	2127.330	1361.666	1531.330	549.936	2133.059	-55.709
2100	1098.334	2180.743	1399.406	1640.806	552.829	2212.140	-55.023
2200	1104.799	2231.989	1436.094	1750.969	555.571	2291.090	-54.396
2300	1110.558	2281.229	1471.776	1861.743	558.155	2369.918	-53.821
2400	1115.706	2328.605	1506.496	1973.060	560.504	2448.584	-53.291
2500	1120.324	2374.246	1540.299	2084.866	562.630	2527.283	-52.804
2600	1124.481	2418.268	1573.226	2197.110	564.491	2605.773	-52.350
2700	1128.234	2460.778	1605.315	2309.749	566.094	2684.275	-51.929
2800	1131.632	2501.871	1636.605	2422.745	567.409	2762.749	-51.539
2900	1134.717	2541.636	1667.131	2536.065	568.403	2841.120	-51.173
3000	1137.527	2580.153	1696.927	2649.679	569.125	2919.492	-50.832
3100	1140.092	2617.495	1726.023	2763.562	569.487	2997.761	-50.511
3200	1142.439	2653.729	1754.451	2877.690	569.538	3076.104	-50.211
3300	1144.592	2688.917	1782.237	2992.043	569.255	3154.494	-49.930
3400	1146.571	2723.116	1809.410	3106.603	568.608	3232.803	-49.665
3500	1148.394	2756.379	1835.993	3221.352	567.603	3311.115	-49.415
3600	1150.077	2788.754	1862.011	3336.277	566.262	3389.557	-49.180
3700	1151.633	2820.287	1887.486	3451.363	564.553	3468.062	-48.959
3800	1153.076	2851.018	1912.439	3566.600	562.444	3546.549	-48.750
3900	1154.415	2880.988	1936.891	3681.975	559.983	3625.041	-48.551
4000	1155.659	2910.231	1960.861	3797.480	557.149	3703.754	-48.365
4100	1156.819	2938.781	1984.366	3913.104	553.905	3782.460	-48.188
4200	1157.900	2966.671	2007.423	4028.841	550.280	3861.241	-48.021
4300	1158.911	2993.929	2030.049	4144.682	546.259	3940.013	-47.861
4400	1159.856	3020.583	2052.260	4260.621	541.853	4018.985	-47.710
4500	1160.742	3046.658	2074.069	4376.651	537.077	4098.125	-47.569
4600	1161.572	3072.179	2095.490	4492.767	531.873	4177.382	-47.435
4700	1162.353	3097.168	2116.538	4608.964	526.257	4256.631	-47.306
4800	1163.087	3121.648	2137.224	4725.236	520.283	4336.121	-47.186
4900	1163.778	3145.637	2157.559	4841.580	513.866	4415.590	-47.070
5000	1164.429	3169.155	2177.557	4957.990	507.112	4495.402	-46.962

3.487. Naphtho[2,1-*a*]pentaphene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-86-9
Point Group: C_s

Length: 18.46 Å
Width: 10.94 Å
Breadth: 3.886 Å
L/B Ratio: 1.688

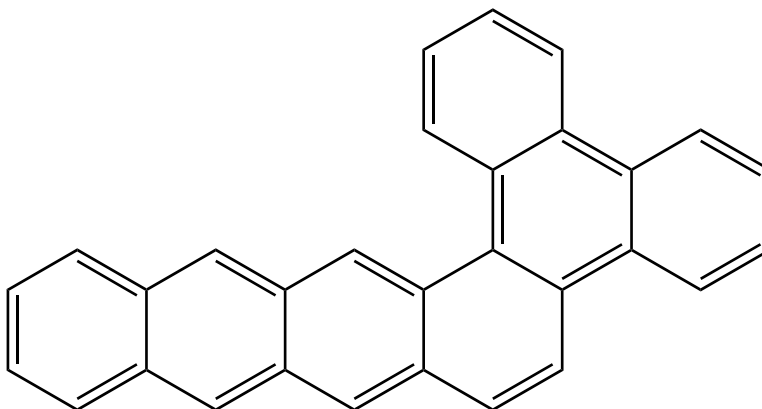
Cartesian coordinates:

C	5.6575	-3.2935	0.0000	C	-1.1309	0.7708	0.0000	H	7.4306	-0.3697	0.0000
C	6.7682	-2.4104	0.0000	C	-1.2935	2.1738	0.0000	H	3.5200	-3.4787	0.0000
C	6.5785	-1.0587	0.0000	C	-2.6143	2.7306	0.0000	H	5.8997	1.5545	0.0000
C	4.3834	-2.8040	0.0000	C	-3.7041	1.9238	0.0000	H	1.9801	-1.5482	0.0000
C	4.1529	-1.3967	0.0000	C	-2.3002	-0.0767	0.0000	H	4.4049	3.4687	0.0000
C	5.2594	-0.5166	0.0000	C	-3.5712	0.4970	0.0000	H	2.1132	4.4097	0.0000
C	5.0378	0.8757	0.0000	C	-3.2605	-2.3063	0.0000	H	-0.2972	4.0959	0.0000
C	2.8469	-0.8675	0.0000	C	-2.1670	-1.4992	0.0000	H	0.2995	-0.8627	0.0000
C	2.6336	0.5001	0.0000	C	-4.5752	-1.7466	0.0000	H	-2.7207	3.8214	0.0000
C	3.7507	1.3849	0.0000	C	-4.7362	-0.3484	0.0000	H	-4.7226	2.3418	0.0000
C	3.5253	2.8143	0.0000	C	-6.0472	0.1881	0.0000	H	-3.1546	-3.3972	0.0000
C	2.2795	3.3261	0.0000	C	-7.1424	-0.6385	0.0000	H	-1.1494	-1.9196	0.0000
C	1.2868	1.0572	0.0000	C	-6.9768	-2.0379	0.0000	H	-6.1636	1.2826	0.0000
C	1.1161	2.4665	0.0000	C	-5.7175	-2.5836	0.0000	H	-8.1533	-0.2181	0.0000
C	-0.1625	3.0070	0.0000	H	5.8404	-4.3731	0.0000	H	-7.8615	-2.6827	0.0000
C	0.1678	0.2364	0.0000	H	7.7788	-2.8319	0.0000	H	-5.5797	-3.6708	0.0000

Table 3.487: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*a*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.591	487.992	487.992	∞
100	127.543	389.048	884.703	-49.565	517.368	571.974	-298.762
200	247.869	512.281	667.781	-31.100	501.808	632.785	-165.263
250	318.027	575.070	642.933	-16.966	494.498	666.376	-139.229
298.15	386.506	636.954	636.954	0.000	487.992	700.086	-122.650
300	389.106	639.353	636.962	0.717	487.752	701.400	-122.122
350	457.504	704.523	641.952	21.900	481.764	737.495	-110.063
400	520.971	769.820	653.857	46.385	476.576	774.382	-101.122
450	578.498	834.563	670.347	73.897	472.099	811.881	-94.239
500	629.953	898.229	689.962	104.133	468.237	849.869	-88.783
600	716.329	1021.029	734.999	171.618	462.021	926.814	-80.685
700	784.755	1136.789	784.215	246.801	457.572	1004.661	-74.967
800	839.736	1245.296	835.143	328.122	454.686	1083.019	-70.712
900	884.622	1346.880	886.421	414.413	453.161	1161.649	-67.419
1000	921.763	1442.067	937.277	504.789	452.811	1240.399	-64.790
1100	952.822	1531.420	987.271	598.564	453.414	1319.146	-62.640
1200	979.013	1615.481	1036.154	695.192	454.811	1397.782	-60.843
1300	1001.255	1694.745	1083.796	794.235	456.795	1476.289	-59.317
1400	1020.259	1769.660	1130.135	895.335	459.219	1554.631	-58.003
1500	1036.589	1840.621	1175.156	998.198	461.989	1632.788	-56.858
1600	1050.695	1907.983	1218.871	1102.579	464.962	1710.743	-55.849
1700	1062.940	1972.057	1261.307	1208.275	468.052	1788.481	-54.952
1800	1073.621	2033.122	1302.502	1315.115	471.176	1866.108	-54.152
1900	1082.979	2091.426	1342.502	1422.955	474.298	1943.502	-53.429
2000	1091.216	2147.189	1381.352	1531.673	477.356	2020.762	-52.776
2100	1098.494	2200.609	1419.102	1641.166	480.265	2097.856	-52.180
2200	1104.952	2251.863	1455.798	1751.345	483.023	2174.820	-51.636
2300	1110.704	2301.110	1491.487	1862.133	485.622	2251.659	-51.136
2400	1115.846	2348.491	1526.214	1973.465	487.985	2328.338	-50.674
2500	1120.457	2394.138	1560.024	2085.284	490.124	2405.048	-50.250
2600	1124.608	2438.165	1592.957	2197.541	491.999	2481.548	-49.854
2700	1128.354	2480.680	1625.053	2310.192	493.614	2558.060	-49.488
2800	1131.746	2521.777	1656.349	2423.200	494.941	2634.543	-49.147
2900	1134.827	2561.547	1686.881	2536.531	495.946	2710.924	-48.828
3000	1137.631	2600.067	1716.681	2650.156	496.678	2787.305	-48.530
3100	1140.191	2637.412	1745.783	2764.049	497.051	2863.582	-48.250
3200	1142.533	2673.649	1774.216	2878.187	497.111	2939.933	-47.988
3300	1144.682	2708.840	1802.007	2992.550	496.837	3016.331	-47.744
3400	1146.657	2743.042	1829.184	3107.118	496.200	3092.647	-47.512
3500	1148.476	2776.307	1855.771	3221.876	495.203	3168.967	-47.293
3600	1150.155	2808.685	1881.794	3336.808	493.870	3245.416	-47.089
3700	1151.708	2840.219	1907.273	3451.903	492.168	3321.927	-46.896
3800	1153.147	2870.953	1932.230	3567.146	490.067	3398.421	-46.714
3900	1154.483	2900.924	1956.686	3682.529	487.613	3474.920	-46.540
4000	1155.725	2930.169	1980.659	3798.040	484.786	3551.639	-46.379
4100	1156.882	2958.721	2004.167	3913.671	481.548	3628.352	-46.225
4200	1157.961	2986.612	2027.228	4029.414	477.930	3705.138	-46.079
4300	1158.969	3013.871	2049.857	4145.261	473.915	3781.916	-45.940
4400	1159.912	3040.526	2072.071	4261.205	469.514	3858.894	-45.810
4500	1160.795	3066.603	2093.883	4377.241	464.743	3936.039	-45.687
4600	1161.624	3092.125	2115.307	4493.363	459.544	4013.302	-45.572
4700	1162.402	3117.116	2136.357	4609.564	453.934	4090.556	-45.460
4800	1163.134	3141.596	2157.046	4725.841	447.964	4168.051	-45.357
4900	1163.824	3165.586	2177.384	4842.190	441.553	4245.525	-45.257
5000	1164.473	3189.105	2197.384	4958.605	434.803	4323.342	-45.165

3.488. Phenanthro[9,10-*a*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115791-73-6
Point Group: C₁

Length: 18.04 Å
Width: 10.40 Å
Breadth: 5.374 Å
L/B Ratio: 1.736

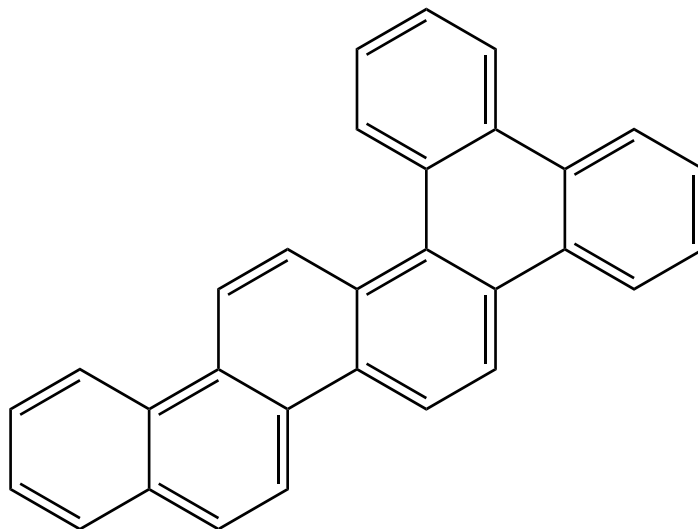
Cartesian coordinates:

C	1.1386	-2.2779	0.7738	C	-0.3467	1.8673	0.4567	H	7.4646	0.1648	-1.1446
C	1.9419	-1.2100	0.3180	C	0.0345	0.5040	0.2139	H	5.8710	-1.7094	-0.7642
C	3.2903	-1.4899	0.0193	C	-1.6758	2.2393	0.4954	H	-7.8178	-1.8968	-0.8661
C	3.7576	-2.8200	0.0612	C	-2.7012	1.3001	0.2388	H	-8.4534	0.4144	-0.2563
C	2.9343	-3.8496	0.4562	C	-2.3350	-0.0312	-0.0942	H	-6.7118	2.1038	0.2868
C	1.6181	-3.5675	0.8419	C	-0.9666	-0.3949	-0.1031	H	-5.4265	-2.5724	-0.9440
C	4.2100	-0.4102	-0.2703	C	-4.0616	1.6615	0.2769	H	-4.3382	2.6896	0.5413
C	3.7750	0.9165	-0.1267	C	-5.0456	0.7294	-0.0181	H	-3.0568	-1.9951	-0.6683
C	2.3809	1.1856	0.1625	C	-4.6786	-0.6062	-0.3669	H	-1.9511	3.2810	0.7036
C	1.4529	0.1575	0.2299	C	-3.3401	-0.9693	-0.4015	H	-0.7201	-1.4332	-0.3699
C	4.7031	1.9621	-0.3230	C	-6.4403	1.0772	0.0158	H	0.3755	3.8991	0.8125
C	6.0061	1.6956	-0.6794	C	-7.3901	0.1547	-0.2806	H	2.7524	3.3232	0.4090
C	6.4300	0.3702	-0.8514	C	-7.0227	-1.1813	-0.6324	H	4.8039	-3.0199	-0.2164
C	5.5457	-0.6647	-0.6458	C	-5.7179	-1.5508	-0.6749	H	3.3045	-4.8792	0.4871
C	1.9715	2.5483	0.3828	H	4.3703	3.0024	-0.1917	H	0.9729	-4.3765	1.2000
C	0.6777	2.8702	0.5858	H	6.7156	2.5153	-0.8326	H	0.1051	-2.0820	1.0911

Table 3.488: Table of thermodynamic data as a function of temperature for Phenanthro[9,10-*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.366	541.622	541.622	∞
100	126.738	379.096	874.380	-49.528	571.035	626.636	-327.314
200	247.746	502.035	657.542	-31.101	555.436	688.463	-179.804
250	318.046	564.813	632.690	-16.969	548.124	722.566	-150.969
298.15	386.647	626.711	626.711	0.000	541.622	756.770	-132.580
300	389.252	629.110	626.718	0.718	541.382	758.103	-131.995
350	457.763	694.311	631.711	21.910	535.404	794.710	-118.601
400	521.319	759.649	643.622	46.411	530.231	832.106	-108.660
450	578.907	824.436	660.121	73.942	525.774	870.113	-100.998
500	630.395	888.148	679.749	104.199	521.933	908.606	-94.919
600	716.773	1011.029	724.814	171.729	515.762	986.554	-85.885
700	785.149	1126.855	774.062	246.955	511.355	1065.398	-79.499
800	840.061	1235.410	825.021	328.312	508.505	1144.747	-74.743
900	884.878	1337.029	876.327	414.632	507.009	1224.364	-71.059
1000	921.959	1432.239	927.209	505.030	506.682	1304.097	-68.118
1100	952.967	1521.608	977.225	598.821	507.302	1383.826	-65.711
1200	979.118	1605.680	1026.128	695.462	508.711	1463.443	-63.701
1300	1001.329	1684.952	1073.787	794.514	510.704	1542.930	-61.994
1400	1020.309	1759.871	1120.142	895.620	513.134	1622.251	-60.526
1500	1036.621	1830.835	1165.177	998.487	515.909	1701.387	-59.246
1600	1050.713	1898.198	1208.904	1102.870	518.883	1780.320	-58.120
1700	1062.948	1962.273	1251.350	1208.568	521.974	1859.037	-57.120
1800	1073.621	2023.338	1292.556	1315.408	525.099	1937.642	-56.228
1900	1082.974	2081.642	1332.564	1423.248	528.220	2016.014	-55.423
2000	1091.206	2137.405	1371.422	1531.965	531.278	2094.253	-54.695
2100	1098.481	2190.824	1409.178	1641.457	534.186	2172.326	-54.033
2200	1104.937	2242.078	1445.880	1751.634	536.942	2250.268	-53.427
2300	1110.687	2291.323	1481.575	1862.421	539.540	2328.086	-52.871
2400	1115.828	2338.704	1516.308	1973.751	541.901	2405.743	-52.359
2500	1120.439	2384.350	1550.122	2085.569	544.039	2483.431	-51.887
2600	1124.589	2428.377	1583.060	2197.824	545.912	2560.910	-51.448
2700	1128.335	2470.890	1615.160	2310.473	547.525	2638.401	-51.042
2800	1131.728	2511.988	1646.459	2423.479	548.850	2715.864	-50.664
2900	1134.808	2551.756	1676.994	2536.808	549.853	2793.224	-50.310
3000	1137.613	2590.276	1706.799	2650.432	550.583	2870.583	-49.980
3100	1140.173	2627.620	1735.903	2764.323	550.955	2947.840	-49.670
3200	1142.516	2663.857	1764.338	2878.459	551.013	3025.170	-49.380
3300	1144.665	2699.047	1792.132	2992.820	550.737	3102.547	-49.108
3400	1146.640	2733.249	1819.312	3107.386	550.098	3179.843	-48.851
3500	1148.460	2766.514	1845.901	3222.142	549.099	3257.142	-48.609
3600	1150.140	2798.891	1871.926	3337.074	547.765	3334.570	-48.382
3700	1151.693	2830.425	1897.407	3452.166	546.062	3412.061	-48.169
3800	1153.133	2861.158	1922.366	3567.408	543.959	3489.534	-47.966
3900	1154.469	2891.128	1946.823	3682.789	541.503	3567.013	-47.774
4000	1155.712	2920.373	1970.798	3798.299	538.675	3644.712	-47.594
4100	1156.869	2948.925	1994.308	3913.929	535.436	3722.404	-47.423
4200	1157.948	2976.816	2017.370	4029.670	531.816	3800.170	-47.261
4300	1158.957	3004.075	2040.001	4145.516	527.800	3877.927	-47.107
4400	1159.900	3030.729	2062.216	4261.460	523.398	3955.885	-46.961
4500	1160.784	3056.806	2084.029	4377.494	518.626	4034.010	-46.825
4600	1161.613	3082.328	2105.455	4493.615	513.426	4112.252	-46.695
4700	1162.392	3107.318	2126.506	4609.815	507.815	4190.486	-46.571
4800	1163.124	3131.798	2147.196	4726.091	501.844	4268.961	-46.455
4900	1163.814	3155.788	2167.535	4842.439	495.431	4347.415	-46.343
5000	1164.464	3179.307	2187.536	4958.853	488.680	4426.212	-46.239

3.489. Dibenzo[*a,c*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-70-1
Point Group: C₁

Length: 17.96 Å
Width: 10.46 Å
Breadth: 5.030 Å
L/B Ratio: 1.717

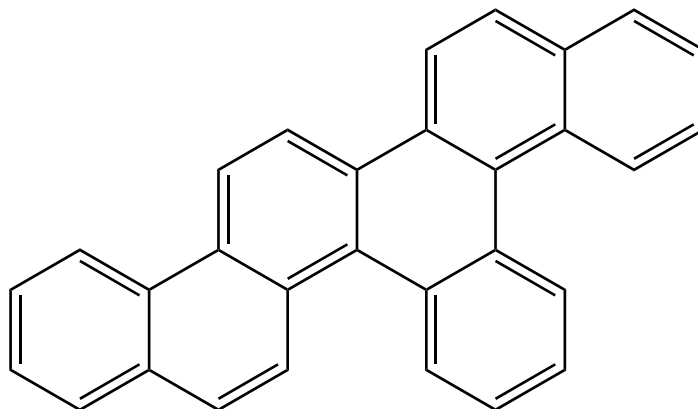
Cartesian coordinates:

C	6.4202	1.5587	0.5633	C	-1.3519	0.1171	-0.1177	H	7.1038	-1.6579	-0.3440
C	7.1678	0.4092	0.2432	C	-1.9573	-1.1423	-0.1521	H	4.4500	2.4109	0.7882
C	6.5290	-0.7588	-0.0947	C	-2.2134	1.2917	-0.2065	H	5.0387	-2.9116	-0.7143
C	5.0477	1.5211	0.5383	C	-3.5990	1.1629	0.0147	H	2.5594	-3.0105	-0.7632
C	4.3658	0.3308	0.1911	C	-4.4243	2.3033	-0.0217	H	0.1963	2.2522	0.6644
C	5.1157	-0.8162	-0.1252	C	-3.9116	3.5420	-0.3421	H	2.6536	2.3187	0.7994
C	4.4379	-2.0274	-0.4723	C	-2.5557	3.6610	-0.6603	H	0.7984	-3.1165	-0.6478
C	3.0814	-2.0781	-0.5001	C	-1.7300	2.5575	-0.5947	H	-1.6694	-3.2780	-0.4413
C	2.9269	0.2659	0.1531	C	-4.1890	-0.1482	0.2074	H	-5.4967	2.1867	0.1979
C	2.2882	-0.9264	-0.1912	C	-3.3891	-1.2893	0.0452	H	-4.5609	4.4228	-0.3670
C	0.7767	1.3588	0.3965	C	-3.9899	-2.5610	0.1346	H	-2.1510	4.6322	-0.9635
C	2.1334	1.4027	0.4785	C	-5.3348	-2.6921	0.4089	H	-0.6703	2.6763	-0.8589
C	0.0822	0.1773	-0.0087	C	-6.1243	-1.5523	0.6030	H	-3.3680	-3.4567	-0.0125
C	0.8505	-0.9827	-0.2271	C	-5.5586	-0.2993	0.4991	H	-5.7886	-3.6859	0.4796
C	0.1916	-2.2215	-0.4433	H	6.9435	2.4819	0.8325	H	-7.1895	-1.6603	0.8317
C	-1.1647	-2.3041	-0.3512	H	8.2614	0.4564	0.2672	H	-6.1738	0.6031	0.6343

Table 3.489: Table of thermodynamic data as a function of temperature for Dibenzo[*a,c*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.260	509.781	509.781	∞
100	127.250	378.728	872.632	-49.390	539.333	594.970	-310.774
200	246.934	501.588	656.501	-30.983	523.714	656.830	-171.543
250	316.797	564.134	631.745	-16.903	516.350	690.962	-144.366
298.15	385.159	625.789	625.789	0.000	509.781	725.204	-127.050
300	387.758	628.179	625.796	0.715	509.539	726.539	-126.499
350	456.183	693.142	630.770	21.830	503.483	763.198	-113.899
400	519.756	758.268	642.639	46.252	498.232	800.658	-104.553
450	577.413	822.876	659.084	73.706	493.697	838.739	-97.356
500	628.990	886.434	678.651	103.891	489.784	877.314	-91.650
600	715.545	1009.076	723.593	171.290	483.482	955.446	-83.177
700	784.064	1124.723	772.724	246.400	478.960	1034.494	-77.193
800	839.083	1233.141	823.574	327.654	476.007	1114.063	-72.739
900	883.986	1334.650	874.782	413.880	474.417	1193.913	-69.291
1000	921.138	1429.769	925.576	504.193	474.004	1273.889	-66.540
1100	952.209	1519.063	975.513	597.906	474.546	1353.869	-64.289
1200	978.416	1603.072	1024.344	694.473	475.881	1433.743	-62.408
1300	1000.679	1682.289	1071.937	793.458	477.807	1513.494	-60.812
1400	1019.708	1757.162	1118.233	894.502	480.174	1593.083	-59.437
1500	1036.064	1828.087	1163.213	997.310	482.891	1672.493	-58.240
1600	1050.197	1895.415	1206.889	1101.640	485.812	1751.702	-57.186
1700	1062.469	1959.459	1249.290	1207.288	488.854	1830.699	-56.249
1800	1073.176	2020.498	1290.453	1314.082	491.932	1909.586	-55.414
1900	1082.561	2078.779	1330.421	1421.879	495.011	1988.244	-54.660
2000	1090.821	2134.521	1369.243	1530.557	498.029	2066.770	-53.977
2100	1098.123	2187.923	1406.965	1640.011	500.899	2145.132	-53.356
2200	1104.603	2239.160	1443.636	1750.154	503.621	2223.365	-52.788
2300	1110.375	2288.391	1479.301	1860.908	506.186	2301.475	-52.267
2400	1115.536	2335.760	1514.006	1972.209	508.518	2379.426	-51.786
2500	1120.165	2381.394	1547.795	2083.998	510.627	2457.410	-51.344
2600	1124.332	2425.410	1580.707	2196.226	512.473	2535.185	-50.931
2700	1128.094	2467.914	1612.784	2308.851	514.062	2612.973	-50.550
2800	1131.501	2509.003	1644.063	2421.833	515.363	2690.734	-50.195
2900	1134.594	2548.764	1674.577	2535.140	516.344	2768.393	-49.863
3000	1137.411	2587.276	1704.362	2648.743	517.054	2846.052	-49.553
3100	1139.982	2624.614	1733.448	2762.614	517.405	2923.609	-49.261
3200	1142.335	2660.845	1761.866	2876.732	517.445	3001.240	-48.989
3300	1144.494	2696.030	1789.644	2991.075	517.152	3078.918	-48.734
3400	1146.478	2730.227	1816.807	3105.625	516.496	3156.516	-48.493
3500	1148.306	2763.487	1843.382	3220.365	515.481	3234.117	-48.266
3600	1149.993	2795.860	1869.393	3335.282	514.132	3311.849	-48.053
3700	1151.554	2827.390	1894.860	3450.360	512.415	3389.643	-47.852
3800	1153.000	2858.119	1919.806	3565.588	510.298	3467.420	-47.662
3900	1154.342	2888.086	1944.252	3680.956	507.829	3545.202	-47.482
4000	1155.591	2917.328	1968.214	3796.454	504.989	3623.205	-47.313
4100	1156.753	2945.877	1991.713	3912.072	501.738	3701.202	-47.153
4200	1157.838	2973.765	2014.764	4027.802	498.107	3779.273	-47.001
4300	1158.851	3001.021	2037.385	4143.637	494.080	3857.336	-46.856
4400	1159.799	3027.674	2059.590	4259.570	489.668	3935.599	-46.721
4500	1160.686	3053.748	2081.394	4375.595	484.885	4014.029	-46.593
4600	1161.519	3079.268	2102.810	4491.705	479.676	4092.577	-46.472
4700	1162.302	3104.256	2123.852	4607.897	474.056	4171.118	-46.356
4800	1163.038	3128.734	2144.533	4724.164	468.076	4249.899	-46.247
4900	1163.731	3152.722	2164.865	4840.503	461.655	4328.659	-46.143
5000	1164.384	3176.240	2184.858	4956.909	454.896	4407.763	-46.047

3.490. Dibenzo[*c,s*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-50-7
Point Group: C₁

Length: 18.09 Å
Width: 10.51 Å
Breadth: 4.855 Å
L/B Ratio: 1.721

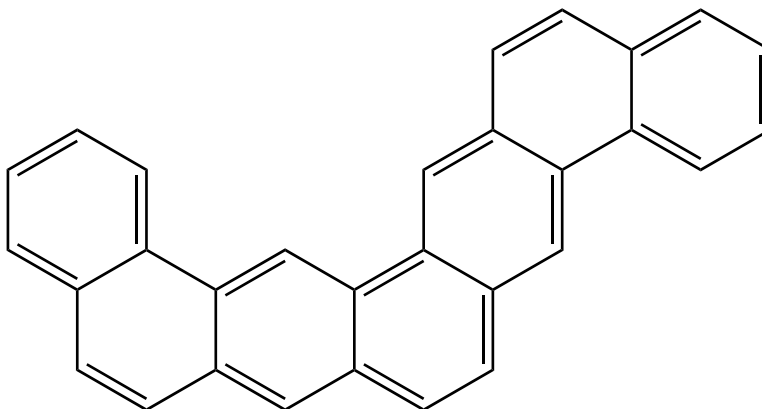
Cartesian coordinates:

C	-6.0903	0.3726	-0.5223	C	0.4991	0.2866	-0.0133	H	-6.0307	-2.8801	0.4691
C	-6.5716	-0.8965	-0.1503	C	-0.0838	-0.9851	-0.0020	H	-4.4053	1.6463	-0.7871
C	-5.6811	-1.8741	0.2100	C	0.7354	-2.1366	-0.1535	H	-3.7736	-3.6692	0.7073
C	-4.7483	0.6536	-0.4660	C	2.0887	-2.0286	-0.2662	H	-1.3425	-3.3007	0.4606
C	-3.8002	-0.3080	-0.0296	C	1.9327	0.3775	0.0932	H	1.1259	2.8555	-0.7365
C	-4.2902	-1.6050	0.2358	C	2.7190	-0.7696	-0.1040	H	-0.3235	4.8325	-0.5482
C	-3.3785	-2.6744	0.4720	C	3.9659	1.6600	0.5453	H	-2.6547	4.5810	0.3158
C	-2.0437	-2.4598	0.3543	C	2.6135	1.5795	0.4851	H	-3.5979	2.3347	0.6416
C	-2.3780	-0.0545	0.0718	C	4.7823	0.5342	0.2117	H	0.2620	-3.1283	-0.2010
C	-1.5187	-1.1502	0.1262	C	4.1613	-0.6868	-0.0993	H	2.7167	-2.9144	-0.4464
C	-1.7837	1.2714	0.0860	C	4.9736	-1.8051	-0.3996	H	4.4597	2.5872	0.8586
C	-0.3915	1.4320	-0.1023	C	6.3436	-1.6971	-0.3985	H	2.0173	2.4565	0.7717
C	0.0858	2.7260	-0.4078	C	6.9593	-0.4699	-0.0919	H	4.4845	-2.7626	-0.6341
C	-0.7164	3.8398	-0.3062	C	6.1922	0.6295	0.2114	H	6.9659	-2.5661	-0.6364
C	-2.0366	3.6960	0.1343	H	-6.7982	1.1347	-0.8649	H	8.0518	-0.3995	-0.0958
C	-2.5544	2.4334	0.3128	H	-7.6475	-1.0963	-0.1716	H	6.6624	1.5889	0.4553

Table 3.490: Table of thermodynamic data as a function of temperature for Dibenzo[*c,s*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.820	550.043	550.043	∞
100	125.318	372.477	864.285	-49.181	579.804	636.066	-332.240
200	245.924	494.340	648.898	-30.912	564.047	698.613	-182.455
250	316.085	556.693	624.193	-16.875	556.640	733.111	-153.172
298.15	384.705	618.245	618.245	0.000	550.043	767.714	-134.498
300	387.313	620.633	618.252	0.714	549.800	769.064	-133.903
350	455.960	685.544	623.222	21.813	543.727	806.102	-120.302
400	519.703	750.653	635.083	46.228	538.469	843.942	-110.205
450	577.483	815.261	651.521	73.683	533.936	882.403	-102.425
500	629.143	878.832	671.084	103.874	530.028	921.359	-96.252
600	715.782	1001.510	716.023	171.292	523.746	1000.250	-87.078
700	784.320	1117.196	765.157	246.427	519.249	1080.053	-80.593
800	839.331	1225.648	816.014	327.707	516.321	1160.373	-75.763
900	884.213	1327.184	867.232	413.957	514.756	1240.970	-72.023
1000	921.341	1422.327	918.035	504.292	514.364	1321.692	-69.037
1100	952.389	1511.639	967.981	598.023	514.925	1402.415	-66.594
1200	978.575	1595.662	1016.822	694.608	516.277	1483.031	-64.553
1300	1000.820	1674.892	1064.425	793.607	518.218	1563.522	-62.822
1400	1019.832	1749.774	1110.729	894.664	520.599	1643.851	-61.332
1500	1036.174	1820.707	1155.717	997.485	523.327	1723.998	-60.034
1600	1050.295	1888.041	1199.401	1101.825	526.259	1803.946	-58.892
1700	1062.557	1952.092	1241.808	1207.482	529.309	1883.679	-57.877
1800	1073.255	2013.135	1282.978	1314.284	532.396	1963.303	-56.972
1900	1082.632	2071.420	1322.952	1422.089	535.482	2042.697	-56.157
2000	1090.886	2127.166	1361.779	1530.773	538.507	2121.959	-55.419
2100	1098.182	2180.571	1399.507	1640.234	541.384	2201.056	-54.747
2200	1104.657	2231.811	1436.182	1750.382	544.111	2280.024	-54.134
2300	1110.425	2281.044	1471.852	1861.142	546.682	2358.869	-53.571
2400	1115.582	2328.414	1506.562	1972.447	549.018	2437.555	-53.051
2500	1120.208	2374.050	1540.354	2084.241	551.131	2516.273	-52.574
2600	1124.371	2418.068	1573.271	2196.473	552.982	2594.782	-52.129
2700	1128.130	2460.574	1605.351	2309.101	554.574	2673.305	-51.717
2800	1131.534	2501.664	1636.633	2422.087	555.879	2751.799	-51.334
2900	1134.626	2541.426	1667.151	2535.398	556.863	2830.192	-50.976
3000	1137.440	2579.939	1696.938	2649.003	557.576	2908.585	-50.642
3100	1140.010	2617.278	1726.028	2762.878	557.930	2986.875	-50.327
3200	1142.361	2653.510	1754.448	2876.998	557.973	3065.240	-50.034
3300	1144.518	2688.696	1782.228	2991.343	557.682	3143.652	-49.759
3400	1146.501	2722.893	1809.394	3105.896	557.028	3221.983	-49.499
3500	1148.327	2756.154	1835.971	3220.638	556.016	3300.318	-49.254
3600	1150.014	2788.527	1861.984	3335.556	554.669	3378.782	-49.024
3700	1151.573	2820.058	1887.453	3450.637	552.953	3457.310	-48.807
3800	1153.018	2850.788	1912.402	3565.867	550.839	3535.820	-48.602
3900	1154.360	2880.755	1936.849	3681.237	548.372	3614.335	-48.408
4000	1155.607	2909.997	1960.813	3796.736	545.533	3693.072	-48.226
4100	1156.769	2938.547	1984.314	3912.356	542.283	3771.801	-48.052
4200	1157.853	2966.435	2007.367	4028.087	538.654	3850.606	-47.888
4300	1158.865	2993.692	2029.989	4143.924	534.628	3929.401	-47.732
4400	1159.812	3020.345	2052.195	4259.858	530.218	4008.397	-47.585
4500	1160.700	3046.419	2074.000	4375.884	525.437	4087.560	-47.446
4600	1161.532	3071.939	2095.418	4491.996	520.229	4166.842	-47.315
4700	1162.314	3096.928	2116.462	4608.189	514.610	4246.115	-47.189
4800	1163.049	3121.406	2137.144	4724.457	508.631	4325.629	-47.071
4900	1163.742	3145.395	2157.477	4840.797	502.211	4405.122	-46.958
5000	1164.394	3168.912	2177.471	4957.204	495.453	4484.958	-46.853

3.491. Dibenzo[*a,m*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-83-6
Point Group: C_s

Length: 18.50 Å
Width: 10.75 Å
Breadth: 3.885 Å
L/B Ratio: 1.722

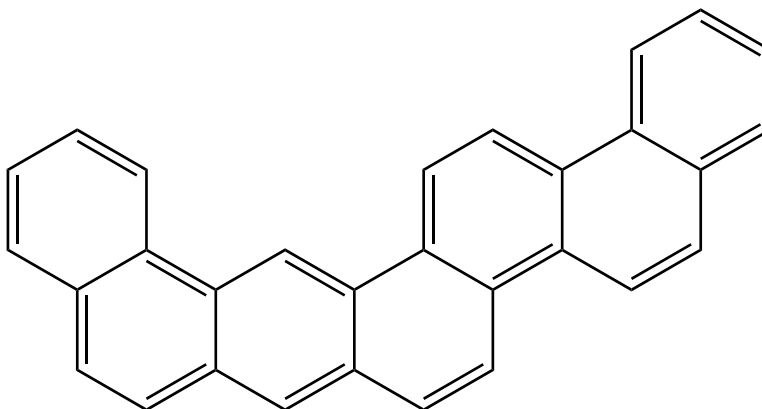
Cartesian coordinates:

C	6.1412	-2.8850	0.0000	C	-0.5238	0.6526	0.0000	H	2.7503	-2.4627	0.0000
C	6.5345	-1.5641	0.0000	C	-1.4469	1.7264	0.0000	H	4.4763	-4.2679	0.0000
C	3.8244	-2.2208	0.0000	C	-2.8150	1.4628	0.0000	H	7.0484	1.0698	0.0000
C	4.7777	-3.2153	0.0000	C	-1.0001	-0.6571	0.0000	H	5.3627	2.8913	0.0000
C	4.2047	-0.8638	0.0000	C	-2.3729	-0.9232	0.0000	H	3.0387	3.6179	0.0000
C	5.5712	-0.5352	0.0000	C	-3.2944	0.1489	0.0000	H	1.5094	-1.1371	0.0000
C	5.9753	0.8465	0.0000	C	-4.1837	-2.5430	0.0000	H	0.7308	4.3846	0.0000
C	5.0570	1.8387	0.0000	C	-2.8578	-2.2792	0.0000	H	-1.7000	3.8946	0.0000
C	3.2167	0.1968	0.0000	C	-5.1498	-1.4757	0.0000	H	-3.5424	2.2909	0.0000
C	3.6475	1.5431	0.0000	C	-4.7152	-0.1390	0.0000	H	-0.2743	-1.4867	0.0000
C	2.7016	2.5737	0.0000	C	-5.6734	0.8944	0.0000	H	-4.5548	-3.5744	0.0000
C	1.8469	-0.0827	0.0000	C	-7.0197	0.6016	0.0000	H	-2.1204	-3.0901	0.0000
C	0.9013	0.9403	0.0000	C	-7.4511	-0.7333	0.0000	H	-5.3188	1.9366	0.0000
C	1.3374	2.2874	0.0000	C	-6.5305	-1.7590	0.0000	H	-7.7592	1.4089	0.0000
C	0.3623	3.3522	0.0000	H	6.8901	-3.6838	0.0000	H	-8.5234	-0.9542	0.0000
C	-0.9603	3.0857	0.0000	H	7.5986	-1.3018	0.0000	H	-6.8632	-2.8033	0.0000

Table 3.491: Table of thermodynamic data as a function of temperature for Dibenzo[*a,m*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.359	476.120	476.120	∞
100	126.899	380.443	875.457	-49.501	505.561	561.027	-293.044
200	247.574	503.332	658.750	-31.084	489.953	622.720	-162.634
250	317.868	566.071	633.912	-16.960	482.632	656.760	-137.220
298.15	386.438	627.935	627.935	0.000	476.120	690.903	-121.041
300	389.041	630.333	627.942	0.717	475.881	692.234	-120.526
350	457.502	695.498	632.932	21.898	469.890	728.781	-108.762
400	521.009	760.797	644.837	46.384	464.704	766.118	-100.043
450	578.562	825.547	661.326	73.899	460.230	804.069	-93.332
500	630.032	889.220	680.943	104.139	456.371	842.508	-88.014
600	716.424	1012.036	725.982	171.632	450.164	920.352	-80.122
700	784.856	1127.812	775.204	246.826	445.725	999.098	-74.552
800	839.838	1236.332	826.137	328.157	442.849	1078.353	-70.408
900	884.724	1337.929	877.420	414.458	441.334	1157.879	-67.200
1000	921.863	1433.126	928.282	504.844	440.994	1237.523	-64.640
1100	952.919	1522.488	978.281	598.628	441.608	1317.164	-62.546
1200	979.106	1606.557	1027.169	695.266	443.013	1396.693	-60.795
1300	1001.344	1685.829	1074.816	794.318	445.006	1476.092	-59.309
1400	1020.344	1760.750	1121.160	895.427	447.439	1555.324	-58.029
1500	1036.669	1831.717	1166.186	998.298	450.218	1634.373	-56.913
1600	1050.770	1899.084	1209.905	1102.686	453.198	1713.218	-55.930
1700	1063.010	1963.162	1252.345	1208.389	456.295	1791.846	-55.056
1800	1073.686	2024.231	1293.544	1315.236	459.426	1870.361	-54.275
1900	1083.041	2082.538	1333.547	1423.083	462.554	1948.644	-53.571
2000	1091.273	2138.305	1372.401	1531.807	465.619	2026.793	-52.933
2100	1098.548	2191.728	1410.154	1641.306	468.533	2104.776	-52.352
2200	1105.003	2242.984	1446.853	1751.489	471.296	2182.627	-51.821
2300	1110.752	2292.233	1482.545	1862.283	473.900	2260.354	-51.333
2400	1115.890	2339.617	1517.275	1973.619	476.268	2337.920	-50.882
2500	1120.499	2385.265	1551.087	2085.443	478.412	2415.518	-50.468
2600	1124.647	2429.294	1584.023	2197.704	480.290	2492.905	-50.082
2700	1128.391	2471.809	1616.121	2310.359	481.910	2570.304	-49.724
2800	1131.782	2512.909	1647.419	2423.370	483.240	2647.674	-49.392
2900	1134.860	2552.679	1677.953	2536.705	484.249	2724.942	-49.080
3000	1137.662	2591.200	1707.756	2650.333	484.984	2802.209	-48.790
3100	1140.221	2628.547	1736.860	2764.229	485.360	2879.373	-48.516
3200	1142.562	2664.785	1765.294	2878.370	485.423	2956.611	-48.261
3300	1144.709	2699.976	1793.087	2992.735	485.152	3033.895	-48.022
3400	1146.682	2734.179	1820.266	3107.306	484.517	3111.098	-47.795
3500	1148.500	2767.445	1846.855	3222.066	483.522	3188.304	-47.582
3600	1150.178	2799.823	1872.878	3337.001	482.192	3265.639	-47.382
3700	1151.730	2831.358	1898.359	3452.098	480.492	3343.037	-47.194
3800	1153.168	2862.092	1923.318	3567.344	478.393	3420.417	-47.016
3900	1154.503	2892.064	1947.775	3682.728	475.941	3497.801	-46.847
4000	1155.744	2921.309	1971.749	3798.241	473.116	3575.407	-46.689
4100	1156.900	2949.862	1995.259	3913.874	469.880	3653.005	-46.539
4200	1157.979	2977.754	2018.321	4029.619	466.263	3730.677	-46.397
4300	1158.986	3005.013	2040.951	4145.468	462.250	3808.341	-46.261
4400	1159.928	3031.669	2063.166	4261.414	457.851	3886.205	-46.134
4500	1160.811	3057.746	2084.979	4377.451	453.082	3964.235	-46.015
4600	1161.639	3083.268	2106.404	4493.574	447.885	4042.384	-45.902
4700	1162.417	3108.259	2127.455	4609.777	442.276	4120.524	-45.794
4800	1163.148	3132.740	2148.145	4726.056	436.307	4198.905	-45.692
4900	1163.837	3156.730	2168.484	4842.406	429.897	4277.264	-45.595
5000	1164.486	3180.249	2188.485	4958.822	423.148	4355.967	-45.506

3.492. Naphtho[1,2-*b*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-82-5
Point Group: C_s

Length: 18.45 Å
Width: 10.50 Å
Breadth: 3.885 Å
L/B Ratio: 1.757

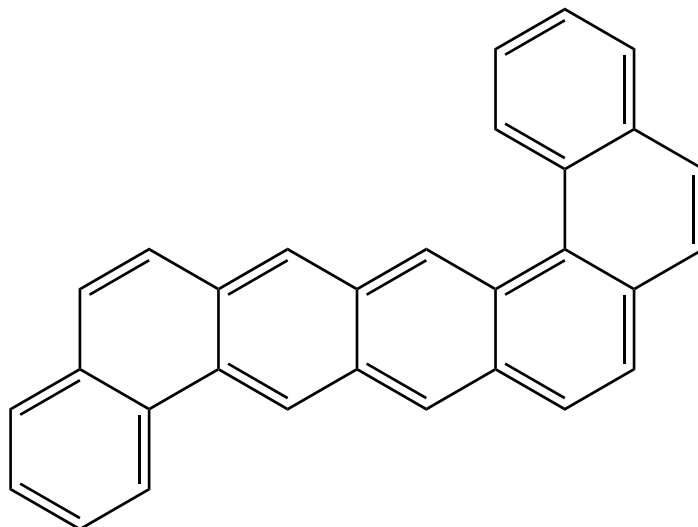
Cartesian coordinates:

C	6.4312	-2.7026	0.0000	C	-0.4868	0.3162	0.0000	H	3.0184	-2.5448	0.0000
C	6.7205	-1.3543	0.0000	C	-1.4858	1.2945	0.0000	H	4.8790	-4.2102	0.0000
C	4.0702	-2.2193	0.0000	C	-2.1648	-1.4300	0.0000	H	7.0301	1.3103	0.0000
C	5.0984	-3.1375	0.0000	C	-0.8522	-1.0559	0.0000	H	5.2102	2.9971	0.0000
C	4.3438	-0.8377	0.0000	C	-3.1986	-0.4564	0.0000	H	2.8357	3.5419	0.0000
C	5.6806	-0.4042	0.0000	C	-2.8631	0.9037	0.0000	H	1.6817	-1.3185	0.0000
C	5.9771	1.0058	0.0000	C	-3.9107	1.8830	0.0000	H	0.4664	4.1215	0.0000
C	4.9863	1.9241	0.0000	C	-5.2164	1.5177	0.0000	H	-1.9182	3.4301	0.0000
C	3.2745	0.1433	0.0000	C	-4.5868	-0.8534	0.0000	H	-2.4518	-2.4929	0.0000
C	3.6017	1.5223	0.0000	C	-5.5880	0.1341	0.0000	H	-0.0482	-1.8081	0.0000
C	2.5833	2.4741	0.0000	C	-6.9488	-0.2482	0.0000	H	-3.6212	2.9449	0.0000
C	1.9353	-0.2409	0.0000	C	-7.2956	-1.5784	0.0000	H	-6.0122	2.2713	0.0000
C	0.9073	0.7073	0.0000	C	-6.2970	-2.5692	0.0000	H	-7.7210	0.5294	0.0000
C	1.2403	2.0825	0.0000	C	-4.9693	-2.2145	0.0000	H	-8.3491	-1.8764	0.0000
C	0.1884	3.0612	0.0000	H	7.2403	-3.4402	0.0000	H	-6.5868	-3.6250	0.0000
C	-1.1107	2.6822	0.0000	H	7.7611	-1.0104	0.0000	H	-4.1786	-2.9803	0.0000

Table 3.492: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*b*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.179	481.151	481.151	∞
100	126.721	381.825	874.652	-49.283	510.810	566.138	-295.714
200	246.406	504.253	658.938	-30.937	495.130	627.713	-163.938
250	316.356	566.693	634.217	-16.881	487.742	661.714	-138.255
298.15	384.671	628.268	628.268	0.000	481.151	695.834	-121.905
300	387.266	630.656	628.276	0.714	480.908	697.165	-121.385
350	455.563	695.533	633.243	21.801	474.824	733.703	-109.497
400	519.000	760.568	645.096	46.189	469.539	771.045	-100.686
450	576.552	825.080	661.518	73.603	464.964	809.013	-93.906
500	628.067	888.544	681.058	103.743	461.006	847.481	-88.534
600	714.614	1011.015	725.936	171.047	454.609	925.410	-80.562
700	783.218	1126.524	774.998	246.068	449.998	1004.272	-74.938
800	838.361	1234.837	825.782	327.244	446.967	1083.667	-70.755
900	883.389	1336.267	876.929	413.404	445.311	1163.351	-67.518
1000	920.653	1431.330	927.667	503.663	444.844	1243.168	-64.935
1100	951.818	1520.582	977.553	597.332	445.342	1322.994	-62.822
1200	978.104	1604.560	1026.340	693.865	446.643	1402.718	-61.057
1300	1000.429	1683.756	1073.893	792.821	448.540	1482.321	-59.559
1400	1019.507	1758.612	1120.153	893.842	450.885	1561.765	-58.269
1500	1035.903	1829.524	1165.101	996.633	453.584	1641.030	-57.145
1600	1050.066	1896.842	1208.749	1100.949	456.491	1720.097	-56.154
1700	1062.363	1960.880	1251.124	1206.584	459.520	1798.951	-55.274
1800	1073.090	2021.913	1292.264	1313.369	462.589	1877.696	-54.488
1900	1082.491	2080.190	1332.212	1421.158	465.660	1956.213	-53.779
2000	1090.764	2135.929	1371.014	1529.830	468.672	2034.598	-53.137
2100	1098.076	2189.328	1408.719	1639.279	471.537	2112.819	-52.552
2200	1104.564	2240.563	1445.374	1749.417	474.254	2190.912	-52.018
2300	1110.344	2289.793	1481.024	1860.168	476.816	2268.882	-51.527
2400	1115.510	2337.160	1515.716	1971.466	479.145	2346.693	-51.073
2500	1120.144	2382.793	1549.492	2083.252	481.251	2424.537	-50.657
2600	1124.314	2426.808	1582.393	2195.479	483.096	2502.172	-50.268
2700	1128.079	2469.312	1614.460	2308.102	484.683	2579.820	-49.909
2800	1131.488	2510.400	1645.728	2421.083	485.983	2657.441	-49.574
2900	1134.584	2550.161	1676.233	2534.389	486.963	2734.960	-49.261
3000	1137.403	2588.673	1706.010	2647.990	487.671	2812.479	-48.969
3100	1139.975	2626.011	1735.088	2761.861	488.022	2889.896	-48.693
3200	1142.330	2662.241	1763.498	2875.978	488.061	2967.388	-48.437
3300	1144.489	2697.426	1791.268	2990.321	487.768	3044.927	-48.196
3400	1146.474	2731.623	1818.425	3104.870	487.111	3122.385	-47.969
3500	1148.303	2764.883	1844.994	3219.610	486.096	3199.847	-47.754
3600	1149.991	2797.255	1870.998	3334.526	484.747	3277.438	-47.553
3700	1151.552	2828.786	1896.460	3449.604	483.029	3355.093	-47.364
3800	1152.999	2859.515	1921.401	3564.833	480.913	3432.730	-47.185
3900	1154.342	2889.482	1945.841	3680.201	478.444	3510.373	-47.015
4000	1155.590	2918.724	1969.799	3795.698	475.603	3588.237	-46.857
4100	1156.753	2947.273	1993.293	3911.316	472.352	3666.094	-46.706
4200	1157.838	2975.161	2016.340	4027.046	468.721	3744.026	-46.563
4300	1158.851	3002.417	2038.956	4142.881	464.694	3821.949	-46.427
4400	1159.799	3029.070	2061.157	4258.814	460.282	3900.072	-46.299
4500	1160.687	3055.144	2082.957	4374.839	455.500	3978.363	-46.179
4600	1161.520	3080.663	2104.370	4490.950	450.291	4056.772	-46.065
4700	1162.303	3105.652	2125.409	4607.141	444.670	4135.172	-45.956
4800	1163.039	3130.130	2146.087	4723.409	438.691	4213.814	-45.855
4900	1163.732	3154.118	2166.415	4839.748	432.270	4292.434	-45.757
5000	1164.385	3177.635	2186.405	4956.154	425.511	4371.399	-45.667

3.493. Benzo[*a*]naphtho[1,2-*j*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 112498-94-9
Point Group: C₁

Length: 18.30 Å
Width: 10.33 Å
Breadth: 5.039 Å
L/B Ratio: 1.772

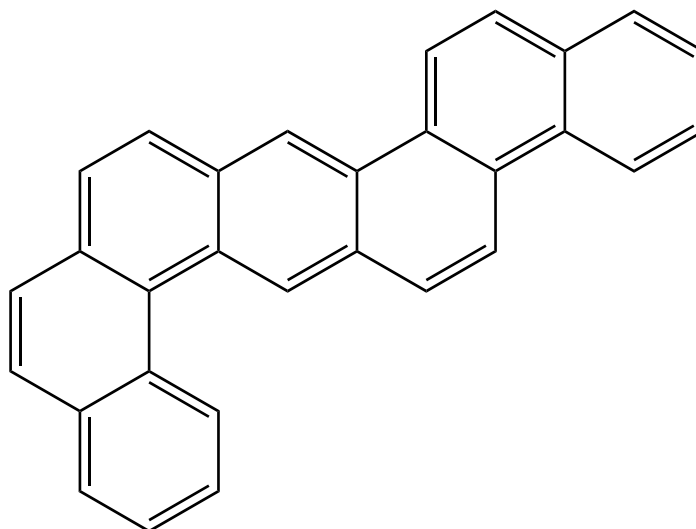
Cartesian coordinates:

C	6.9002	-0.9060	0.0690	C	-1.7930	0.6890	0.0043	H	7.1874	2.4186	-0.5756
C	7.4962	0.3141	-0.1854	C	-1.1901	1.9814	-0.1436	H	4.6997	2.2553	-0.4542
C	6.7083	1.4550	-0.3745	C	-2.0191	3.1598	-0.1432	H	3.0584	-3.3671	0.6772
C	5.3318	1.3659	-0.3077	C	-3.3459	3.0571	0.0741	H	5.5250	-3.1549	0.5494
C	5.5002	-1.0104	0.1395	C	-3.2498	0.5900	0.0141	H	2.8948	2.1088	-0.3505
C	4.7065	0.1334	-0.0501	C	-3.9787	1.7681	0.1806	H	0.8477	-2.3655	0.5562
C	3.5328	-2.3997	0.4751	C	-5.3801	1.7391	0.4404	H	0.6308	3.1147	-0.3509
C	4.8741	-2.2847	0.4057	C	-6.0503	0.5578	0.4789	H	-1.3636	-1.3901	0.4189
C	2.6709	-1.2538	0.2859	C	-3.9892	-0.6417	-0.1335	H	-1.5384	4.1348	-0.2835
C	3.2567	0.0251	0.0229	C	-5.3730	-0.6532	0.1516	H	-3.9780	3.9503	0.1429
C	2.4414	1.1241	-0.1524	C	-6.1147	-1.8585	0.0667	H	-5.9012	2.6858	0.6256
C	1.2991	-1.3858	0.3552	C	-5.5167	-3.0161	-0.3574	H	-7.1180	0.5199	0.7234
C	0.4537	-0.2651	0.1662	C	-4.1597	-2.9982	-0.7331	H	-7.1774	-1.8459	0.3354
C	1.0334	1.0038	-0.0792	C	-3.4227	-1.8466	-0.6256	H	-6.0844	-3.9496	-0.4235
C	0.1853	2.1215	-0.2126	H	7.5147	-1.8012	0.2177	H	-3.6990	-3.9134	-1.1196
C	-0.9515	-0.3920	0.2100	H	8.5868	0.3932	-0.2400	H	-2.3722	-1.8583	-0.9467

Table 3.493: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[1,2-*j*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.037	519.672	519.672	∞
100	125.304	376.863	869.912	-49.305	549.309	605.133	-316.082
200	246.631	498.839	653.913	-31.015	533.573	667.239	-174.261
250	317.182	561.397	629.125	-16.932	526.212	701.508	-146.569
298.15	385.935	623.157	623.157	0.000	519.672	735.879	-128.920
300	388.544	625.553	623.165	0.716	519.431	737.219	-128.359
350	457.145	690.651	628.149	21.876	513.420	774.006	-115.512
400	520.758	755.910	640.043	46.347	508.218	811.587	-105.980
450	578.390	820.635	656.520	73.851	503.733	849.783	-98.638
500	629.919	884.294	676.125	104.084	499.868	888.467	-92.816
600	716.383	1007.096	721.146	171.570	493.653	966.805	-84.166
700	784.849	1122.868	770.352	246.761	489.212	1046.045	-78.055
800	839.845	1231.389	821.273	328.092	486.336	1125.795	-73.505
900	884.735	1332.986	872.548	414.394	484.822	1205.815	-69.982
1000	921.873	1428.184	923.403	504.782	484.483	1285.953	-67.170
1100	952.927	1517.547	973.396	598.567	485.098	1366.088	-64.869
1200	979.111	1601.617	1022.280	695.205	486.504	1446.111	-62.946
1300	1001.346	1680.890	1069.922	794.258	488.497	1526.004	-61.314
1400	1020.344	1755.811	1116.263	895.367	490.930	1605.731	-59.909
1500	1036.668	1826.778	1161.286	998.237	493.709	1685.273	-58.685
1600	1050.767	1894.144	1205.003	1102.626	496.689	1764.612	-57.607
1700	1063.007	1958.222	1247.440	1208.329	499.786	1843.734	-56.650
1800	1073.682	2019.291	1288.638	1315.175	502.916	1922.744	-55.795
1900	1083.036	2077.598	1328.639	1423.021	506.044	2001.521	-55.025
2000	1091.268	2133.364	1367.492	1531.745	509.108	2080.163	-54.327
2100	1098.543	2186.787	1405.243	1641.243	512.022	2158.640	-53.692
2200	1104.998	2238.043	1441.940	1751.427	514.784	2236.986	-53.112
2300	1110.747	2287.292	1477.631	1862.219	517.388	2315.207	-52.579
2400	1115.885	2334.675	1512.360	1973.556	519.755	2393.267	-52.087
2500	1120.494	2380.323	1546.171	2085.379	521.898	2471.359	-51.635
2600	1124.642	2424.352	1579.106	2197.639	523.777	2549.240	-51.214
2700	1128.387	2466.867	1611.203	2310.294	525.395	2627.134	-50.824
2800	1131.777	2507.966	1642.501	2423.305	526.725	2704.998	-50.461
2900	1134.855	2547.737	1673.034	2536.639	527.733	2782.760	-50.122
3000	1137.658	2586.258	1702.836	2650.266	528.468	2860.521	-49.805
3100	1140.216	2623.604	1731.939	2764.162	528.844	2938.180	-49.507
3200	1142.557	2659.842	1760.372	2878.302	528.906	3015.912	-49.229
3300	1144.705	2695.033	1788.165	2992.667	528.635	3093.690	-48.968
3400	1146.678	2729.236	1815.343	3107.238	527.999	3171.387	-48.721
3500	1148.496	2762.502	1841.931	3221.998	527.004	3249.087	-48.489
3600	1150.175	2794.880	1867.954	3336.932	525.674	3326.917	-48.271
3700	1151.727	2826.415	1893.434	3452.028	523.974	3404.809	-48.066
3800	1153.165	2857.149	1918.393	3567.274	521.875	3482.683	-47.872
3900	1154.500	2887.120	1942.849	3682.658	519.422	3560.562	-47.687
4000	1155.741	2916.366	1966.823	3798.171	516.596	3638.662	-47.515
4100	1156.897	2944.918	1990.332	3913.803	513.360	3716.755	-47.351
4200	1157.976	2972.810	2013.394	4029.548	509.743	3794.921	-47.196
4300	1158.983	3000.069	2036.024	4145.396	505.730	3873.079	-47.048
4400	1159.925	3026.725	2058.238	4261.342	501.331	3951.438	-46.909
4500	1160.808	3052.802	2080.051	4377.379	496.561	4029.963	-46.778
4600	1161.636	3078.324	2101.476	4493.502	491.364	4108.605	-46.654
4700	1162.414	3103.315	2122.527	4609.705	485.755	4187.240	-46.535
4800	1163.146	3127.795	2143.216	4725.983	479.786	4266.115	-46.424
4900	1163.835	3151.786	2163.555	4842.333	473.375	4344.969	-46.317
5000	1164.484	3175.305	2183.555	4958.749	466.626	4424.166	-46.218

3.494. Phenanthro[4,3-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 42851-11-6
Point Group: C₁

Length: 18.30 Å
Width: 10.24 Å
Breadth: 4.927 Å
L/B Ratio: 1.788

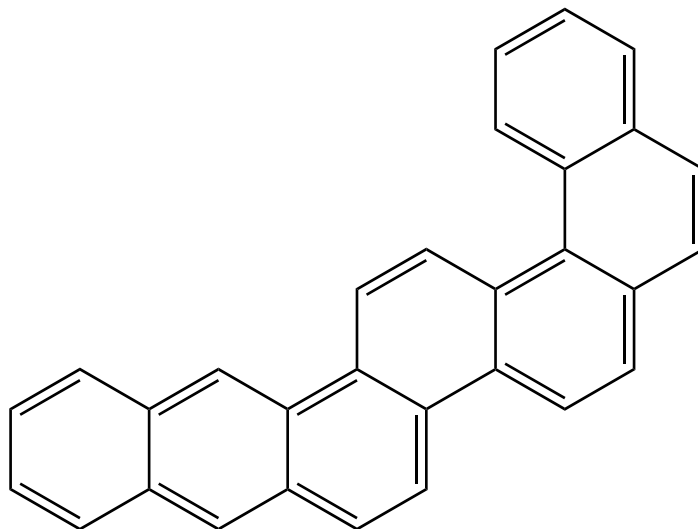
Cartesian coordinates:

C	-6.8162	1.7620	0.2231	C	1.7302	-0.5212	0.0279	H	-7.3159	-1.5487	-0.4309
C	-7.4977	0.5554	-0.0350	C	1.0245	-1.7485	-0.1176	H	-4.9023	2.7199	0.4820
C	-6.7941	-0.6062	-0.2300	C	1.7433	-2.9917	-0.1423	H	-5.1879	-2.7359	-0.5716
C	-5.4460	1.7843	0.2809	C	3.0808	-3.0044	0.0502	H	-2.6973	-2.7225	-0.4703
C	-4.6942	0.5996	0.0827	C	3.1856	-0.5393	0.0207	H	-0.6296	2.7469	0.6443
C	-5.3785	-0.6036	-0.1741	C	3.8182	-1.7771	0.1596	H	-3.1156	2.7257	0.5596
C	-4.6384	-1.8083	-0.3745	C	5.2220	-1.8661	0.4021	H	-0.9047	-2.7200	-0.3169
C	-3.2797	-1.8002	-0.3204	C	5.9857	-0.7450	0.4533	H	1.4710	1.5891	0.4577
C	-3.2569	0.5961	0.1368	C	4.0240	0.6305	-0.1184	H	1.1789	-3.9208	-0.2810
C	-2.5607	-0.5937	-0.0651	C	5.4059	0.5242	0.1536	H	3.6344	-3.9495	0.1003
C	-1.1777	1.8191	0.4436	C	6.2428	1.6650	0.0802	H	5.6657	-2.8556	0.5636
C	-2.5311	1.8067	0.3982	C	5.7386	2.8743	-0.3237	H	7.0552	-0.7973	0.6869
C	-0.4254	0.6143	0.2271	C	4.3836	2.9722	-0.6902	H	7.3031	1.5621	0.3391
C	-1.1153	-0.5974	-0.0142	C	3.5547	1.8830	-0.5904	H	6.3814	3.7585	-0.3810
C	-0.3701	-1.7674	-0.1690	H	-7.3921	2.6804	0.3770	H	3.9967	3.9266	-1.0626
C	0.9719	0.6314	0.2489	H	-8.5917	0.5562	-0.0777	H	2.5069	1.9855	-0.9044

Table 3.494: Table of thermodynamic data as a function of temperature for Phenanthro[4,3-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.285	507.056	507.056	∞
100	126.455	380.569	874.862	-49.429	536.569	592.022	-309.234
200	247.215	503.153	658.427	-31.055	520.917	653.720	-170.731
250	317.578	565.820	633.610	-16.948	513.581	687.771	-143.699
298.15	386.203	627.637	627.637	0.000	507.056	721.928	-126.476
300	388.808	630.034	627.645	0.717	506.816	723.259	-125.928
350	457.327	695.167	632.632	21.887	500.816	759.822	-113.395
400	520.890	760.447	644.531	46.366	495.621	797.176	-104.098
450	578.490	825.185	661.015	73.876	491.143	835.145	-96.939
500	629.994	888.853	680.626	104.113	487.282	873.602	-91.263
600	716.414	1011.665	725.657	171.605	481.072	951.483	-82.832
700	784.837	1127.439	774.872	246.797	476.632	1030.266	-76.878
800	839.793	1235.956	825.800	328.125	473.753	1109.558	-72.445
900	884.650	1337.545	877.078	414.420	472.232	1189.122	-69.013
1000	921.763	1432.733	927.935	504.797	471.884	1268.805	-66.274
1100	952.800	1522.084	977.929	598.571	472.486	1348.486	-64.033
1200	978.974	1606.143	1026.813	695.196	473.879	1428.056	-62.160
1300	1001.204	1685.404	1074.455	794.234	475.858	1507.497	-60.571
1400	1020.200	1760.314	1120.794	895.329	478.277	1586.773	-59.202
1500	1036.525	1831.272	1165.815	998.185	481.041	1665.865	-58.009
1600	1050.628	1898.628	1209.529	1102.560	484.007	1744.755	-56.959
1700	1062.872	1962.698	1251.964	1208.249	487.090	1823.429	-56.026
1800	1073.553	2023.760	1293.158	1315.082	490.207	1901.991	-55.193
1900	1082.913	2082.060	1333.157	1422.916	493.323	1980.322	-54.442
2000	1091.151	2137.820	1372.006	1531.627	496.375	2058.519	-53.762
2100	1098.431	2191.237	1409.754	1641.114	499.277	2136.550	-53.143
2200	1104.892	2242.488	1446.449	1751.286	502.029	2214.451	-52.577
2300	1110.646	2291.732	1482.137	1862.069	504.622	2292.228	-52.057
2400	1115.790	2339.111	1516.863	1973.395	506.979	2369.844	-51.577
2500	1120.404	2384.755	1550.672	2085.209	509.113	2447.492	-51.136
2600	1124.557	2428.781	1583.604	2197.461	510.983	2524.931	-50.725
2700	1128.305	2471.293	1615.698	2310.107	512.593	2602.381	-50.345
2800	1131.700	2512.389	1646.993	2423.110	513.915	2679.803	-49.991
2900	1134.782	2552.157	1677.524	2536.436	514.916	2757.123	-49.660
3000	1137.589	2590.676	1707.323	2650.057	515.643	2834.443	-49.351
3100	1140.150	2628.020	1736.424	2763.946	516.012	2911.659	-49.060
3200	1142.495	2664.255	1764.855	2878.080	516.068	2988.950	-48.789
3300	1144.645	2699.445	1792.646	2992.439	515.791	3066.287	-48.534
3400	1146.621	2733.646	1819.822	3107.003	515.149	3143.543	-48.294
3500	1148.442	2766.910	1846.408	3221.758	514.149	3220.802	-48.067
3600	1150.123	2799.287	1872.429	3336.687	512.813	3298.191	-47.855
3700	1151.678	2830.821	1897.908	3451.778	511.108	3375.642	-47.655
3800	1153.118	2861.553	1922.864	3567.019	509.004	3453.076	-47.465
3900	1154.455	2891.523	1947.319	3682.398	506.546	3530.515	-47.285
4000	1155.698	2920.768	1971.291	3797.907	503.717	3608.174	-47.117
4100	1156.856	2949.319	1994.799	3913.535	500.476	3685.827	-46.957
4200	1157.936	2977.210	2017.859	4029.275	496.855	3763.553	-46.806
4300	1158.945	3004.469	2040.487	4145.120	492.838	3841.272	-46.661
4400	1159.889	3031.123	2062.700	4261.062	488.435	3919.190	-46.526
4500	1160.773	3057.199	2084.511	4377.096	483.662	3997.275	-46.398
4600	1161.603	3082.721	2105.935	4493.215	478.461	4075.478	-46.278
4700	1162.382	3107.711	2126.984	4609.414	472.849	4153.673	-46.162
4800	1163.115	3132.191	2147.672	4725.690	466.877	4232.109	-46.054
4900	1163.805	3156.180	2168.010	4842.036	460.463	4310.523	-45.950
5000	1164.455	3179.699	2188.009	4958.449	453.711	4389.281	-45.854

3.495. Dibenzo[*a,n*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-62-1
Point Group: C₁

Length: 18.29 Å
Width: 10.24 Å
Breadth: 4.826 Å
L/B Ratio: 1.787

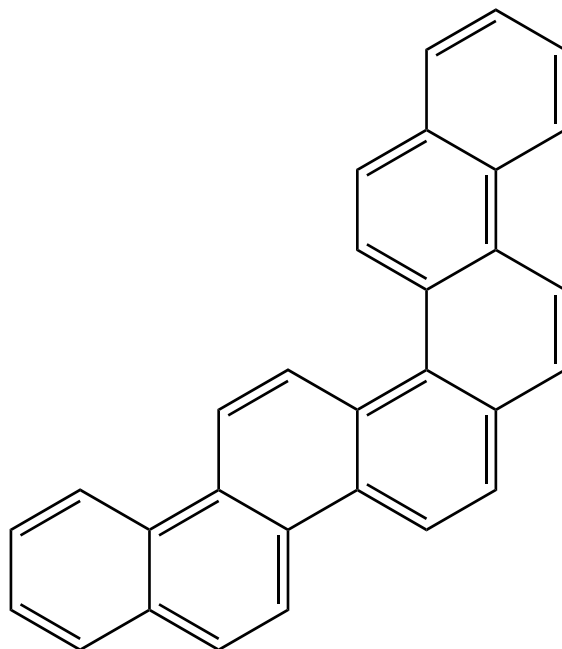
Cartesian coordinates:

C	-6.7314	2.3316	-0.2674	C	1.7243	-0.2929	-0.0903	H	-7.3632	-0.9764	0.3348
C	-7.4607	1.1350	-0.0256	C	0.9731	-1.4771	0.0467	H	-4.8001	3.2293	-0.5146
C	-6.8096	-0.0493	0.1481	C	1.6457	-2.7347	0.0853	H	-5.2534	-2.2366	0.4493
C	-5.3703	2.3122	-0.3288	C	2.9919	-2.8018	-0.0783	H	-2.6842	1.9679	-0.3988
C	-4.6558	1.0871	-0.1508	C	3.1681	-0.3510	-0.0575	H	-3.1665	-3.4958	0.5603
C	-5.3825	-0.1053	0.0897	C	3.7694	-1.6108	-0.1741	H	-0.6936	-3.5691	0.4561
C	-4.6899	-1.3136	0.2644	C	5.1769	-1.7423	-0.3969	H	1.5662	1.8332	-0.5582
C	-3.2544	1.0442	-0.2095	C	5.9713	-0.6461	-0.4489	H	-0.8921	1.8924	-0.5389
C	-2.5685	-0.1521	-0.0342	C	4.0441	0.7954	0.0883	H	1.0470	-3.6489	0.2133
C	-3.3017	-1.3475	0.2047	C	5.4246	0.6451	-0.1656	H	3.5038	-3.7704	-0.1195
C	-2.5852	-2.5839	0.3807	C	6.2956	1.7569	-0.0837	H	5.5916	-2.7464	-0.5439
C	-1.2355	-2.6203	0.3251	C	5.8248	2.9837	0.3131	H	7.0420	-0.7299	-0.6675
C	-1.1202	-0.2147	-0.0861	C	4.4712	3.1245	0.6629	H	7.3555	1.6205	-0.3280
C	-0.4595	-1.4288	0.0954	C	3.6091	2.0601	0.5541	H	6.4952	3.8467	0.3771
C	1.0089	0.9122	-0.3395	H	-7.2840	3.2670	-0.4029	H	4.1086	4.0907	1.0294
C	-0.3545	0.9522	-0.3399	H	-8.5536	1.1839	0.0181	H	2.5612	2.1962	0.8538

Table 3.495: Table of thermodynamic data as a function of temperature for Dibenzo[*a,n*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.099	514.474	514.474	∞
100	125.758	377.806	871.230	-49.342	544.073	599.803	-313.299
200	246.814	500.045	655.126	-31.016	528.374	661.798	-172.840
250	317.186	562.624	630.338	-16.929	521.017	696.006	-145.420
298.15	385.805	624.372	624.372	0.000	514.474	730.319	-127.946
300	388.410	626.767	624.380	0.716	514.233	731.657	-127.390
350	456.917	691.837	629.362	21.866	508.212	768.384	-114.673
400	520.474	757.062	641.250	46.325	502.998	805.906	-105.238
450	578.075	821.751	657.720	73.814	498.498	844.045	-97.972
500	629.587	885.376	677.315	104.030	494.616	882.675	-92.211
600	716.040	1008.116	722.312	171.483	488.368	960.908	-83.653
700	784.502	1123.835	771.493	246.639	483.892	1040.048	-77.608
800	839.498	1232.310	822.390	327.936	480.982	1119.703	-73.108
900	884.390	1333.866	873.640	414.203	479.433	1199.634	-69.623
1000	921.535	1429.028	924.472	504.556	479.060	1279.686	-66.843
1100	952.598	1518.360	974.443	598.308	479.641	1359.738	-64.567
1200	978.795	1602.401	1023.306	694.914	481.015	1439.681	-62.666
1300	1001.045	1681.649	1070.929	793.936	482.978	1519.497	-61.053
1400	1020.058	1756.549	1117.252	895.015	485.381	1599.149	-59.664
1500	1036.398	1827.496	1162.258	997.858	488.132	1678.618	-58.453
1600	1050.513	1894.846	1205.958	1102.221	491.086	1757.886	-57.388
1700	1062.768	1958.909	1248.380	1207.899	494.158	1836.939	-56.441
1800	1073.458	2019.964	1289.563	1314.722	497.265	1915.880	-55.596
1900	1082.826	2078.260	1329.551	1422.547	500.371	1994.591	-54.834
2000	1091.072	2134.016	1368.390	1531.250	503.415	2073.168	-54.144
2100	1098.359	2187.429	1406.129	1640.729	506.310	2151.580	-53.517
2200	1104.825	2238.677	1442.816	1750.895	509.054	2229.862	-52.943
2300	1110.584	2287.918	1478.496	1861.670	511.641	2308.020	-52.416
2400	1115.733	2335.295	1513.215	1972.991	513.993	2386.018	-51.929
2500	1120.351	2380.936	1547.017	2084.799	516.121	2464.048	-51.482
2600	1124.507	2424.960	1579.942	2197.046	517.986	2541.868	-51.066
2700	1128.259	2467.470	1612.031	2309.687	519.591	2619.701	-50.680
2800	1131.657	2508.565	1643.320	2422.686	520.909	2697.505	-50.322
2900	1134.742	2548.331	1673.845	2536.008	521.905	2775.208	-49.986
3000	1137.551	2586.849	1703.640	2649.625	522.629	2852.910	-49.673
3100	1140.115	2624.191	1732.736	2763.510	522.994	2930.509	-49.378
3200	1142.461	2660.426	1761.163	2877.641	523.046	3008.183	-49.103
3300	1144.613	2695.615	1788.949	2991.996	522.766	3085.903	-48.845
3400	1146.591	2729.815	1816.121	3106.557	522.121	3163.542	-48.601
3500	1148.414	2763.078	1842.704	3221.309	521.118	3241.184	-48.371
3600	1150.096	2795.454	1868.722	3336.236	519.779	3318.956	-48.156
3700	1151.652	2826.987	1894.197	3451.324	518.072	3396.791	-47.953
3800	1153.094	2857.719	1919.150	3566.562	515.965	3474.608	-47.761
3900	1154.432	2887.688	1943.601	3681.939	513.505	3552.430	-47.578
4000	1155.676	2916.932	1967.571	3797.445	510.673	3630.474	-47.408
4100	1156.835	2945.483	1991.075	3913.072	507.430	3708.510	-47.246
4200	1157.916	2973.373	2014.133	4028.810	503.808	3786.620	-47.093
4300	1158.926	3000.631	2036.759	4144.652	499.788	3864.722	-46.946
4400	1159.871	3027.285	2058.969	4260.593	495.384	3943.024	-46.809
4500	1160.756	3053.361	2080.778	4376.624	490.608	4021.493	-46.679
4600	1161.586	3078.882	2102.199	4492.742	485.406	4100.080	-46.557
4700	1162.366	3103.872	2123.247	4608.940	479.792	4178.659	-46.440
4800	1163.099	3128.352	2143.932	4725.214	473.818	4257.478	-46.330
4900	1163.790	3152.341	2164.268	4841.558	467.403	4336.276	-46.224
5000	1164.441	3175.859	2184.265	4957.970	460.650	4415.418	-46.127

3.496. Naphtho[2,1-*a*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-51-8
Point Group: C₁

Length: 18.55 Å
Width: 10.28 Å
Breadth: 4.845 Å
L/B Ratio: 1.804

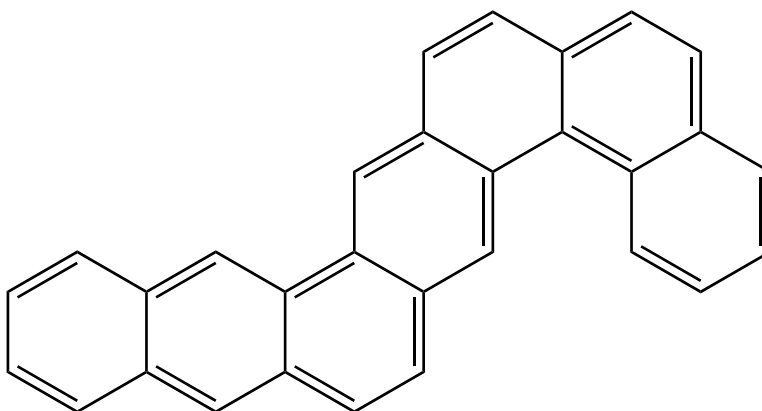
Cartesian coordinates:

C	6.0363	-2.6328	-0.3390	C	-1.0550	0.9203	-0.0061	H	7.5641	0.3333	0.3700
C	7.0659	-1.7112	-0.0720	C	-1.2787	2.3053	-0.0726	H	3.9109	-2.9282	-0.5754
C	6.7678	-0.3905	0.1626	C	-2.5910	2.8254	-0.2557	H	5.9184	2.1278	0.5800
C	4.7265	-2.2194	-0.3653	C	-3.6590	1.9867	-0.3244	H	3.5640	2.9044	0.5376
C	4.3936	-0.8660	-0.1245	C	-2.2106	0.0656	0.1220	H	-0.1344	-1.6004	-0.6204
C	5.4251	0.0525	0.1392	C	-3.4927	0.5912	-0.0999	H	2.2104	-2.3463	-0.6669
C	5.1007	1.4260	0.3794	C	-3.2073	-2.1020	0.6483	H	1.9118	3.4809	0.3298
C	3.8111	1.8473	0.3574	C	-2.1183	-1.2976	0.5566	H	-0.4160	4.3006	0.0486
C	3.0264	-0.4079	-0.1410	C	-4.5058	-1.6151	0.3039	H	-2.7213	3.9092	-0.3565
C	2.7338	0.9368	0.1020	C	-4.6541	-0.2653	-0.0577	H	-4.6722	2.3709	-0.5169
C	0.6634	-0.8833	-0.3838	C	-5.9486	0.2144	-0.3706	H	-3.1122	-3.1375	0.9953
C	1.9589	-1.3032	-0.4198	C	-7.0359	-0.6240	-0.3336	H	-1.1357	-1.6942	0.8467
C	0.3171	0.4640	-0.0726	C	-6.8791	-1.9766	0.0228	H	-6.0657	1.2738	-0.6444
C	1.3686	1.3836	0.0880	C	-5.6351	-2.4657	0.3391	H	-8.0334	-0.2462	-0.5807
C	1.0777	2.7783	0.1833	H	6.2889	-3.6816	-0.5257	H	-7.7560	-2.6317	0.0463
C	-0.1954	3.2267	0.0478	H	8.1046	-2.0567	-0.0539	H	-5.5019	-3.5165	0.6203

Table 3.496: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*a*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.168	505.366	505.366	∞
100	126.136	379.171	872.733	-49.356	534.952	590.545	-308.463
200	246.862	501.555	656.609	-31.011	519.271	652.394	-170.384
250	317.126	564.132	631.827	-16.924	511.914	686.526	-143.439
298.15	385.670	625.863	625.863	0.000	505.366	720.766	-126.273
300	388.273	628.257	625.871	0.716	505.125	722.101	-125.726
350	456.742	693.303	630.851	21.858	499.096	758.755	-113.236
400	520.287	758.503	642.735	46.307	493.872	796.205	-103.972
450	577.890	823.170	659.198	73.787	489.363	834.272	-96.838
500	629.410	886.776	678.786	103.995	485.473	872.831	-91.182
600	715.876	1009.486	723.769	171.430	479.207	950.925	-82.784
700	784.342	1125.179	772.936	246.570	474.715	1029.931	-76.853
800	839.335	1233.633	823.819	327.851	471.789	1109.452	-72.438
900	884.224	1335.170	875.057	414.102	470.224	1189.251	-69.021
1000	921.366	1430.314	925.876	504.438	469.834	1269.174	-66.293
1100	952.430	1519.629	975.836	598.173	470.398	1349.098	-64.062
1200	978.629	1603.657	1024.688	694.762	471.755	1428.915	-62.198
1300	1000.883	1682.891	1072.301	793.767	473.701	1508.606	-60.615
1400	1019.903	1757.779	1118.614	894.831	476.089	1588.135	-59.253
1500	1036.249	1828.716	1163.610	997.659	478.825	1667.482	-58.066
1600	1050.371	1896.056	1207.302	1102.007	481.764	1746.628	-57.020
1700	1062.634	1960.111	1249.716	1207.671	484.822	1825.560	-56.091
1800	1073.332	2021.159	1290.891	1314.482	487.917	1904.382	-55.263
1900	1082.707	2079.448	1330.872	1422.294	491.011	1982.973	-54.515
2000	1090.959	2135.197	1369.705	1530.986	494.042	2061.432	-53.838
2100	1098.253	2188.606	1407.437	1640.453	496.926	2139.726	-53.222
2200	1104.725	2239.849	1444.117	1750.609	499.661	2217.890	-52.658
2300	1110.490	2289.085	1479.792	1861.375	502.238	2295.931	-52.141
2400	1115.644	2336.458	1514.506	1972.686	504.580	2373.813	-51.664
2500	1120.267	2382.096	1548.302	2084.486	506.700	2451.726	-51.225
2600	1124.428	2426.117	1581.223	2196.724	508.556	2529.431	-50.816
2700	1128.185	2468.624	1613.307	2309.358	510.154	2607.148	-50.437
2800	1131.586	2509.716	1644.592	2422.349	511.464	2684.837	-50.085
2900	1134.675	2549.480	1675.113	2535.665	512.454	2762.425	-49.756
3000	1137.487	2587.995	1704.904	2649.275	513.171	2840.012	-49.448
3100	1140.055	2625.336	1733.996	2763.154	513.530	2917.497	-49.158
3200	1142.404	2661.569	1762.419	2877.279	513.577	2995.056	-48.888
3300	1144.559	2696.756	1790.202	2991.629	513.290	3072.662	-48.635
3400	1146.540	2730.954	1817.370	3106.185	512.641	3150.187	-48.396
3500	1148.365	2764.216	1843.950	3220.931	511.632	3227.716	-48.170
3600	1150.049	2796.591	1869.965	3335.853	510.289	3305.374	-47.959
3700	1151.607	2828.122	1895.437	3450.937	508.577	3383.095	-47.760
3800	1153.051	2858.853	1920.387	3566.171	506.466	3460.799	-47.571
3900	1154.391	2888.822	1944.836	3681.544	504.002	3538.507	-47.392
4000	1155.637	2918.064	1968.803	3797.046	501.166	3616.437	-47.225
4100	1156.798	2946.614	1992.305	3912.668	497.919	3694.360	-47.066
4200	1157.880	2974.503	2015.360	4028.403	494.293	3772.357	-46.915
4300	1158.892	3001.761	2037.984	4144.242	490.270	3850.346	-46.771
4400	1159.838	3028.414	2060.192	4260.179	485.862	3928.535	-46.637
4500	1160.724	3054.489	2081.999	4376.208	481.084	4006.891	-46.510
4600	1161.556	3080.010	2103.418	4492.322	475.878	4085.366	-46.390
4700	1162.337	3104.999	2124.463	4608.517	470.261	4163.832	-46.275
4800	1163.071	3129.478	2145.147	4724.788	464.285	4242.538	-46.167
4900	1163.763	3153.467	2165.481	4841.130	457.867	4321.224	-46.064
5000	1164.415	3176.985	2185.477	4957.539	451.111	4400.254	-45.968

3.497. Naphtho[2,1-*c*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115791-75-8
Point Group: C₁

Length: 18.61 Å
Width: 10.14 Å
Breadth: 5.059 Å
L/B Ratio: 1.836

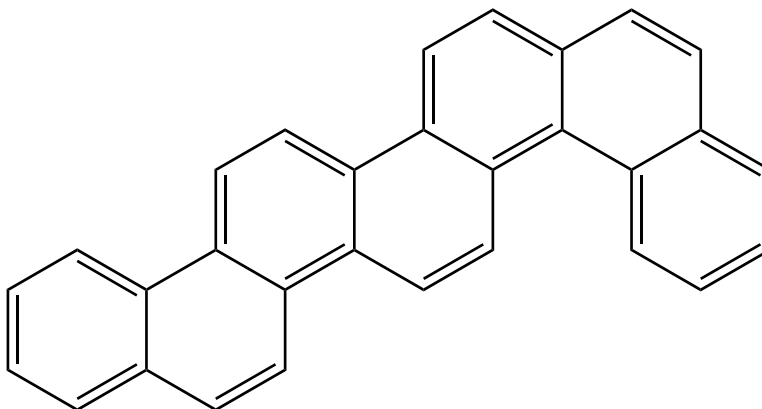
Cartesian coordinates:

C	7.1142	1.4397	-0.4006	C	-0.8000	1.5083	-0.0492	H	7.1196	-1.9294	0.1841
C	7.6076	0.1254	-0.1933	C	-1.6889	0.4096	0.0596	H	5.3819	2.6974	-0.5459
C	6.7470	-0.9115	0.0231	C	-2.6356	3.0694	0.0777	H	4.8167	-2.7555	0.4273
C	5.7718	1.6857	-0.3866	C	-1.3095	2.8471	-0.0768	H	3.0657	1.8704	-0.3018
C	4.8473	0.6230	-0.1632	C	-3.5565	1.9739	0.1518	H	2.5466	-3.5891	0.6795
C	5.3387	-0.6866	0.0436	C	-3.1201	0.6521	0.0168	H	0.1014	-3.1990	0.6969
C	4.4303	-1.7415	0.2659	C	-5.8652	1.2896	0.3851	H	-1.7728	-1.7238	0.4665
C	3.4572	0.8523	-0.1446	C	-4.9366	2.2782	0.3616	H	1.2699	2.1627	-0.1939
C	2.5691	-0.1870	0.0715	C	-5.4824	-0.0538	0.0871	H	-3.0338	4.0898	0.1258
C	3.0664	-1.5056	0.2815	C	-4.1280	-0.3722	-0.1547	H	-0.6024	3.6773	-0.1862
C	2.1335	-2.5876	0.5117	C	-3.8482	-1.6777	-0.6311	H	-6.9193	1.5058	0.5936
C	0.8032	-2.3754	0.5205	C	-4.8342	-2.6243	-0.7613	H	-5.2248	3.3239	0.5215
C	1.1302	0.0375	0.0892	C	-6.1651	-2.3194	-0.4236	H	-2.8224	-1.9396	-0.9240
C	0.2535	-1.0559	0.2963	C	-6.4844	-1.0489	-0.0174	H	-4.5915	-3.6241	-1.1362
C	-1.1211	-0.8572	0.2824	H	7.8286	2.2517	-0.5717	H	-6.9363	-3.0920	-0.5049
C	0.5889	1.3050	-0.0676	H	8.6896	-0.0417	-0.2100	H	-7.5217	-0.7841	0.2183

Table 3.497: Table of thermodynamic data as a function of temperature for Naphtho[2,1-c]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-56.945	510.459	510.459	∞
100	125.081	375.780	868.289	-49.251	540.150	596.082	-311.355
200	246.370	497.632	652.527	-30.979	524.396	658.303	-171.928
250	316.809	560.118	627.767	-16.912	517.019	692.634	-144.715
298.15	385.497	621.806	621.806	0.000	510.459	727.069	-127.377
300	388.105	624.199	621.814	0.716	510.217	728.411	-126.825
350	456.680	689.228	626.793	21.852	504.183	765.268	-114.208
400	520.296	754.425	638.674	46.300	498.958	802.922	-104.849
450	577.946	819.096	655.136	73.782	494.451	841.193	-97.641
500	629.501	882.709	674.723	103.993	490.564	879.956	-91.926
600	716.026	1005.441	719.706	171.441	484.310	958.456	-83.439
700	784.551	1121.162	768.878	246.599	479.837	1037.864	-77.445
800	839.598	1229.647	819.768	327.903	476.934	1117.786	-72.982
900	884.530	1331.217	871.015	414.182	475.397	1197.982	-69.528
1000	921.703	1426.396	921.845	504.551	475.040	1278.298	-66.770
1100	952.783	1515.744	971.816	598.320	475.638	1358.612	-64.514
1200	978.990	1599.802	1020.681	694.946	477.031	1438.816	-62.629
1300	1001.243	1679.066	1068.307	793.987	479.014	1518.891	-61.029
1400	1020.255	1753.980	1114.633	895.086	481.437	1598.801	-59.651
1500	1036.591	1824.941	1159.642	997.949	484.208	1678.527	-58.450
1600	1050.700	1892.303	1203.346	1102.330	487.180	1758.049	-57.393
1700	1062.947	1956.377	1245.773	1208.027	490.271	1837.356	-56.454
1800	1073.630	2017.443	1286.961	1314.868	493.395	1916.550	-55.616
1900	1082.990	2075.747	1326.953	1422.709	496.518	1995.512	-54.859
2000	1091.226	2131.511	1365.797	1531.428	499.578	2074.340	-54.175
2100	1098.505	2184.932	1403.540	1640.922	502.488	2153.002	-53.552
2200	1104.964	2236.186	1440.231	1751.102	505.247	2231.533	-52.982
2300	1110.715	2285.433	1475.915	1861.891	507.847	2309.940	-52.459
2400	1115.857	2332.815	1510.639	1973.225	510.211	2388.186	-51.976
2500	1120.468	2378.462	1544.444	2085.045	512.352	2466.464	-51.533
2600	1124.618	2422.490	1577.373	2197.303	514.228	2544.531	-51.119
2700	1128.364	2465.005	1609.466	2309.955	515.844	2622.611	-50.736
2800	1131.756	2506.103	1640.759	2422.964	517.172	2700.662	-50.380
2900	1134.836	2545.873	1671.288	2536.296	518.178	2778.610	-50.047
3000	1137.640	2584.393	1701.086	2649.922	518.911	2856.558	-49.736
3100	1140.200	2621.739	1730.185	2763.816	519.285	2934.403	-49.443
3200	1142.542	2657.976	1758.615	2877.955	519.346	3012.321	-49.170
3300	1144.690	2693.167	1786.404	2992.318	519.073	3090.286	-48.914
3400	1146.665	2727.369	1813.579	3106.887	518.436	3168.170	-48.672
3500	1148.484	2760.635	1840.165	3221.646	517.439	3246.057	-48.444
3600	1150.163	2793.013	1866.185	3336.579	516.108	3324.073	-48.230
3700	1151.715	2824.547	1891.662	3451.674	514.407	3402.152	-48.029
3800	1153.154	2855.281	1916.618	3566.918	512.306	3480.213	-47.838
3900	1154.490	2885.252	1941.072	3682.301	509.852	3558.279	-47.657
4000	1155.732	2914.497	1965.044	3797.813	507.026	3636.565	-47.488
4100	1156.888	2943.050	1988.551	3913.445	503.789	3714.845	-47.327
4200	1157.967	2970.941	2011.610	4029.188	500.171	3793.198	-47.174
4300	1158.975	2998.200	2034.238	4145.036	496.157	3871.543	-47.029
4400	1159.917	3024.856	2056.451	4260.981	491.757	3950.089	-46.893
4500	1160.801	3050.932	2078.262	4377.017	486.986	4028.800	-46.764
4600	1161.629	3076.454	2099.685	4493.139	481.788	4107.630	-46.643
4700	1162.407	3101.445	2120.734	4609.342	476.178	4186.452	-46.526
4800	1163.139	3125.926	2141.421	4725.619	470.209	4265.514	-46.417
4900	1163.828	3149.916	2161.759	4841.968	463.798	4344.555	-46.313
5000	1164.478	3173.435	2181.758	4958.384	457.048	4423.939	-46.216

3.498. Naphtho[2,1-*c*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-43-8
Point Group: C₁

Length: 18.58 Å
Width: 10.01 Å
Breadth: 4.856 Å
L/B Ratio: 1.857

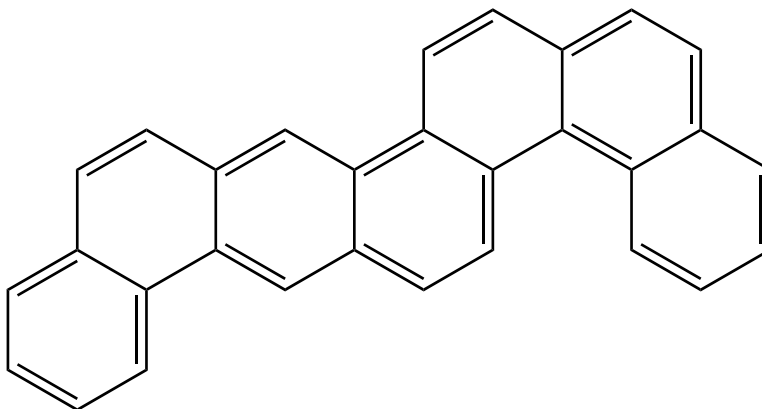
Cartesian coordinates:

C	7.0941	0.8912	0.3420	C	-0.8083	1.2305	0.0109	H	6.9853	-2.4627	-0.2680
C	7.5446	-0.4251	0.1291	C	-1.7333	0.1796	-0.1181	H	5.3844	2.2000	0.4862
C	6.6423	-1.4353	-0.1011	C	-2.6001	2.8504	-0.0367	H	4.6809	-3.2235	-0.5314
C	5.7504	1.1751	0.3213	C	-1.2743	2.5737	0.0849	H	2.2413	-2.7394	-0.5747
C	4.8011	0.1528	0.0869	C	-3.5518	1.7959	-0.1247	H	1.1805	3.0264	0.4076
C	5.2549	-1.1614	-0.1259	C	-3.1472	0.4557	-0.0444	H	3.6229	2.5471	0.4502
C	4.3067	-2.2067	-0.3659	C	-5.8821	1.1835	-0.3537	H	0.4995	-2.3797	-0.6709
C	2.9762	-1.9414	-0.3880	C	-4.9289	2.1442	-0.3064	H	-1.9148	-1.9393	-0.6215
C	3.3852	0.4256	0.0614	C	-5.5327	-0.1820	-0.1049	H	-2.9565	3.8871	-0.0506
C	2.4809	-0.6148	-0.1721	C	-4.1858	-0.5463	0.1086	H	-0.5376	3.3820	0.2062
C	1.5543	2.0036	0.2493	C	-3.9381	-1.8702	0.5440	H	-6.9326	1.4333	-0.5418
C	2.8912	1.7442	0.2708	C	-4.9504	-2.7927	0.6616	H	-5.1883	3.2026	-0.4270
C	0.6072	0.9627	0.0233	C	-6.2743	-2.4403	0.3516	H	-2.9165	-2.1713	0.8127
C	1.0725	-0.3403	-0.1906	C	-6.5612	-1.1483	-0.0145	H	-4.7307	-3.8095	1.0037
C	0.1208	-1.3717	-0.4415	H	7.8246	1.6863	0.5241	H	-7.0679	-3.1910	0.4220
C	-1.2145	-1.1214	-0.4032	H	8.6189	-0.6350	0.1486	H	-7.5937	-0.8473	-0.2271

Table 3.498: Table of thermodynamic data as a function of temperature for Naphtho[2,1-c]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-57.120	504.726	504.726	∞
100	126.187	378.419	871.583	-49.316	534.351	590.020	-308.188
200	246.632	500.743	655.650	-30.981	518.660	651.945	-170.267
250	316.817	563.260	630.892	-16.908	511.290	686.120	-143.354
298.15	385.329	624.933	624.933	0.000	504.726	720.403	-126.209
300	387.931	627.325	624.940	0.715	504.484	721.740	-125.664
350	456.397	692.317	629.917	21.840	498.438	758.442	-113.189
400	519.956	757.472	641.791	46.272	493.197	795.942	-103.937
450	577.581	822.102	658.243	73.736	488.672	834.062	-96.813
500	629.125	885.676	677.818	103.929	484.767	872.675	-91.166
600	715.636	1008.338	722.774	171.338	478.475	950.882	-82.780
700	784.139	1123.998	771.917	246.457	473.961	1030.004	-76.858
800	839.160	1232.425	822.778	327.718	471.016	1109.645	-72.451
900	884.071	1333.943	873.996	413.953	469.434	1189.565	-69.039
1000	921.231	1429.073	924.798	504.275	469.030	1269.612	-66.316
1100	952.309	1518.376	974.742	597.997	469.581	1349.661	-64.089
1200	978.520	1602.393	1023.581	694.574	470.927	1429.604	-62.228
1300	1000.785	1681.619	1071.181	793.569	472.863	1509.422	-60.648
1400	1019.813	1756.500	1117.483	894.624	475.241	1589.077	-59.288
1500	1036.167	1827.431	1162.469	997.443	477.969	1668.553	-58.103
1600	1050.297	1894.766	1206.152	1101.783	480.900	1747.828	-57.060
1700	1062.566	1958.817	1248.558	1207.440	483.951	1826.889	-56.132
1800	1073.269	2019.861	1289.725	1314.244	487.039	1905.840	-55.305
1900	1082.649	2078.146	1329.699	1422.050	490.127	1984.561	-54.558
2000	1090.905	2133.893	1368.525	1530.736	493.153	2063.150	-53.883
2100	1098.203	2187.299	1406.252	1640.199	496.032	2141.575	-53.268
2200	1104.679	2238.540	1442.926	1750.350	498.761	2219.870	-52.705
2300	1110.447	2287.774	1478.596	1861.111	501.334	2298.042	-52.189
2400	1115.604	2335.146	1513.304	1972.419	503.672	2376.055	-51.712
2500	1120.230	2380.782	1547.096	2084.215	505.788	2454.100	-51.275
2600	1124.393	2424.801	1580.013	2196.449	507.641	2531.936	-50.866
2700	1128.152	2467.308	1612.093	2309.080	509.235	2609.785	-50.488
2800	1131.556	2508.398	1643.374	2422.068	510.543	2687.606	-50.137
2900	1134.646	2548.161	1673.892	2535.380	511.529	2765.325	-49.808
3000	1137.460	2586.675	1703.679	2648.988	512.244	2843.044	-49.501
3100	1140.029	2624.015	1732.768	2762.864	512.600	2920.661	-49.212
3200	1142.380	2660.247	1761.189	2876.987	512.644	2998.352	-48.942
3300	1144.536	2695.434	1788.969	2991.334	512.355	3076.091	-48.689
3400	1146.518	2729.631	1816.135	3105.888	511.704	3153.748	-48.450
3500	1148.344	2762.893	1842.712	3220.632	510.693	3231.409	-48.225
3600	1150.030	2795.266	1868.724	3335.552	509.348	3309.199	-48.014
3700	1151.589	2826.798	1894.194	3450.634	507.634	3387.053	-47.816
3800	1153.034	2857.528	1919.142	3565.866	505.521	3464.889	-47.627
3900	1154.375	2887.496	1943.589	3681.237	503.055	3542.730	-47.449
4000	1155.621	2916.738	1967.554	3796.738	500.218	3620.793	-47.282
4100	1156.783	2945.288	1991.054	3912.359	496.969	3698.848	-47.123
4200	1157.866	2973.177	2014.107	4028.092	493.341	3776.978	-46.973
4300	1158.878	3000.434	2036.729	4143.930	489.317	3855.100	-46.829
4400	1159.825	3027.087	2058.936	4259.865	484.908	3933.422	-46.695
4500	1160.711	3053.162	2080.741	4375.893	480.128	4011.910	-46.568
4600	1161.543	3078.682	2102.159	4492.006	474.921	4090.517	-46.448
4700	1162.325	3103.671	2123.203	4608.200	469.303	4169.116	-46.334
4800	1163.060	3128.149	2143.885	4724.469	463.326	4247.956	-46.226
4900	1163.752	3152.138	2164.218	4840.810	456.907	4326.774	-46.123
5000	1164.404	3175.656	2184.212	4957.218	450.150	4405.937	-46.028

3.499. Benzo[*l*]naphtho[1,2-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-42-7
Point Group: C₁

Length: 18.54 Å
Width: 9.878 Å
Breadth: 5.003 Å
L/B Ratio: 1.876

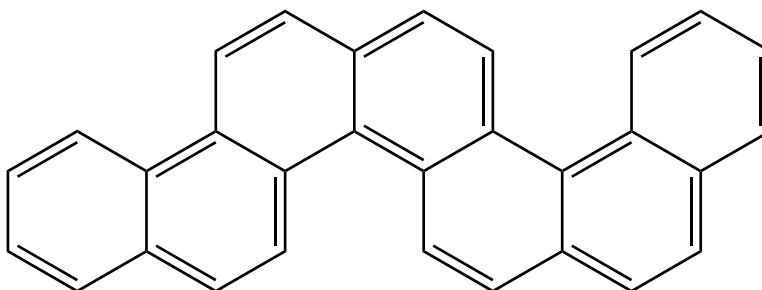
Cartesian coordinates:

C	-7.0513	0.0734	0.2023	C	0.8010	0.9895	-0.0492	H	-6.7551	-3.2606	-0.3841
C	-7.4238	-1.2387	-0.0013	C	1.7995	0.0102	-0.1610	H	-4.3358	-2.6416	-0.4123
C	-6.4492	-2.2217	-0.2234	C	2.4660	2.7362	-0.0630	H	-3.6903	3.2035	0.5519
C	-5.1133	-1.8817	-0.2392	C	1.1594	2.3600	0.0315	H	-6.0832	2.5481	0.5713
C	-5.6904	0.4361	0.1890	C	3.4910	1.7567	-0.1324	H	-2.5854	-2.1627	-0.4327
C	-4.7117	-0.5477	-0.0333	C	3.1838	0.3877	-0.0630	H	-1.3396	2.6153	0.3205
C	-3.9922	2.1621	0.3905	C	5.8642	1.3172	-0.3266	H	-0.2130	-2.7196	-0.7570
C	-5.2951	1.8054	0.4012	C	4.8433	2.2048	-0.2914	H	2.1530	-2.0878	-0.6726
C	-2.9562	1.1845	0.1668	C	5.6118	-0.0724	-0.0875	H	2.7426	3.7970	-0.0723
C	-3.3102	-0.1713	-0.0463	C	4.2928	-0.5353	0.1051	H	0.3603	3.1094	0.1371
C	-2.3044	-1.1104	-0.2647	C	4.1369	-1.8740	0.5360	H	6.8964	1.6436	-0.4969
C	-1.6145	1.5606	0.1589	C	5.2128	-2.7204	0.6668	H	5.0262	3.2798	-0.4050
C	-0.6003	0.6189	-0.0520	C	6.5111	-2.2706	0.3777	H	3.1359	-2.2494	0.7881
C	-0.9587	-0.7309	-0.2709	C	6.7071	-0.9596	0.0173	H	5.0631	-3.7515	1.0040
C	0.0785	-1.6911	-0.5143	H	-7.8103	0.8448	0.3761	H	7.3566	-2.9612	0.4586
C	1.3828	-1.3344	-0.4578	H	-8.4820	-1.5196	0.0092	H	7.7176	-0.5826	-0.1786

Table 3.499: Table of thermodynamic data as a function of temperature for Benzo[*l*]naphtho[1,2-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.917	504.785	504.785	∞
100	125.312	376.349	868.354	-49.200	534.526	590.402	-308.388
200	246.067	498.163	652.849	-30.937	518.763	652.565	-170.429
250	316.374	560.567	628.122	-16.889	511.368	686.871	-143.511
298.15	384.972	622.170	622.170	0.000	504.785	721.286	-126.364
300	387.576	624.560	622.178	0.715	504.542	722.628	-125.818
350	456.100	689.503	627.150	21.823	498.480	759.469	-113.342
400	519.697	754.620	639.016	46.242	493.226	797.111	-104.090
450	577.351	819.221	655.457	73.694	488.688	835.374	-96.966
500	628.920	882.772	675.022	103.875	484.772	874.132	-91.318
600	715.485	1005.401	719.957	171.267	478.462	952.631	-82.932
700	784.046	1121.042	769.081	246.373	473.936	1032.048	-77.011
800	839.124	1229.461	819.927	327.628	470.984	1111.985	-72.604
900	884.083	1330.978	871.132	413.861	469.402	1192.202	-69.192
1000	921.280	1426.111	921.924	504.186	469.001	1272.544	-66.470
1100	952.386	1515.420	971.861	597.915	469.558	1352.890	-64.242
1200	978.616	1599.444	1020.693	694.501	470.913	1433.128	-62.381
1300	1000.893	1678.679	1068.289	793.506	472.859	1513.240	-60.801
1400	1019.928	1753.568	1114.588	894.572	475.249	1593.189	-59.441
1500	1036.285	1824.507	1159.572	997.403	477.988	1672.957	-58.256
1600	1050.415	1891.850	1203.253	1101.755	480.931	1752.525	-57.213
1700	1062.682	1955.907	1245.658	1207.424	483.994	1831.877	-56.286
1800	1073.383	2016.958	1286.826	1314.239	487.093	1911.119	-55.458
1900	1082.759	2075.250	1326.799	1422.056	490.192	1990.130	-54.711
2000	1091.011	2131.002	1365.626	1530.754	493.229	2069.008	-54.036
2100	1098.305	2184.413	1403.353	1640.227	496.118	2147.722	-53.421
2200	1104.776	2235.659	1440.028	1750.387	498.858	2226.305	-52.858
2300	1110.540	2284.897	1475.698	1861.158	501.440	2304.766	-52.342
2400	1115.692	2332.272	1510.408	1972.475	503.787	2383.065	-51.865
2500	1120.314	2377.913	1544.201	2084.279	505.912	2461.398	-51.427
2600	1124.473	2421.935	1577.118	2196.522	507.773	2539.520	-51.019
2700	1128.228	2464.444	1609.200	2309.160	509.375	2617.656	-50.641
2800	1131.628	2505.538	1640.482	2422.156	510.690	2695.763	-50.289
2900	1134.715	2545.303	1671.001	2535.475	511.683	2773.768	-49.960
3000	1137.526	2583.819	1700.789	2649.090	512.404	2851.773	-49.653
3100	1140.091	2621.161	1729.880	2762.972	512.767	2929.676	-49.364
3200	1142.439	2657.395	1758.301	2877.101	512.817	3007.652	-49.094
3300	1144.593	2692.583	1786.082	2991.454	512.534	3085.676	-48.841
3400	1146.572	2726.783	1813.249	3106.013	511.888	3163.618	-48.602
3500	1148.396	2760.046	1839.828	3220.763	510.883	3241.563	-48.377
3600	1150.079	2792.421	1865.841	3335.688	509.543	3319.639	-48.166
3700	1151.636	2823.953	1891.311	3450.775	507.833	3397.777	-47.967
3800	1153.079	2854.685	1916.261	3566.011	505.725	3475.897	-47.779
3900	1154.418	2884.654	1940.709	3681.387	503.264	3554.023	-47.600
4000	1155.663	2913.897	1964.674	3796.892	500.430	3632.369	-47.433
4100	1156.822	2942.448	1988.176	3912.517	497.186	3710.709	-47.274
4200	1157.904	2970.338	2011.230	4028.253	493.562	3789.123	-47.124
4300	1158.914	2997.596	2033.853	4144.095	489.542	3867.528	-46.980
4400	1159.859	3024.250	2056.060	4260.034	485.136	3946.134	-46.846
4500	1160.745	3050.325	2077.866	4376.065	480.360	4024.906	-46.719
4600	1161.576	3075.846	2099.285	4492.181	475.156	4103.797	-46.599
4700	1162.356	3100.836	2120.330	4608.378	469.541	4182.679	-46.484
4800	1163.090	3125.315	2141.013	4724.651	463.567	4261.802	-46.377
4900	1163.781	3149.304	2161.346	4840.995	457.151	4340.904	-46.274
5000	1164.432	3172.822	2181.341	4957.406	450.396	4420.350	-46.178

3.500. Benzo[*c*]naphtho[1,2-*l*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-52-9
Point Group: C₁

Length: 18.12 Å
Width: 9.402 Å
Breadth: 4.800 Å
L/B Ratio: 1.928

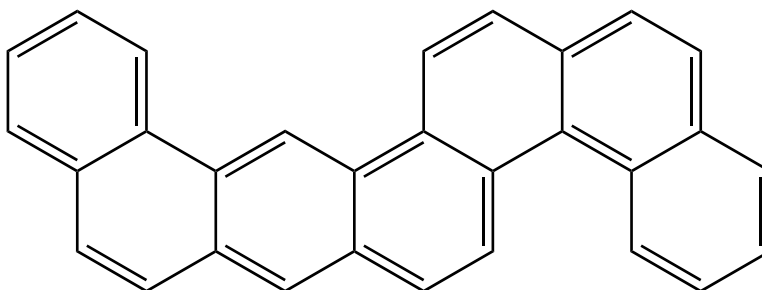
Cartesian coordinates:

C	-5.7639	-1.9744	0.3754	C	0.7289	-1.8934	-0.2082	H	-7.4470	0.8959	-0.3200
C	-6.8445	-1.1251	0.0882	C	0.8477	-0.4988	-0.1044	H	-3.6571	-2.1753	0.6271
C	-6.6124	0.2106	-0.1315	C	3.1002	-2.2051	0.1072	H	-5.9773	2.7856	-0.3399
C	-4.4769	-1.4902	0.3724	C	1.8641	-2.7413	-0.0730	H	-3.7145	3.7507	0.0486
C	-4.1917	-0.1362	0.0757	C	3.2885	-0.7961	0.0273	H	-1.4230	3.4688	0.6520
C	-5.2962	0.7257	-0.0994	C	2.1834	0.0502	-0.1526	H	0.6110	2.0970	0.7275
C	-5.1053	2.1430	-0.1729	C	2.4474	1.4225	-0.4724	H	-0.5837	-3.5566	-0.6975
C	-3.8717	2.6662	0.0200	C	3.7043	1.9348	-0.4800	H	-2.6148	-2.1820	-0.7960
C	-2.8483	0.4167	0.0341	C	4.6259	-0.2556	0.0802	H	3.9800	-2.8445	0.2755
C	-2.7332	1.8083	0.1555	C	4.8290	1.1140	-0.1602	H	1.7187	-3.8275	-0.0953
C	-1.4697	2.3972	0.4248	C	6.1342	1.6558	-0.1035	H	1.6063	2.0729	-0.7480
C	-0.3417	1.6369	0.4328	C	7.2062	0.8475	0.1861	H	3.8802	2.9854	-0.7388
C	-1.6332	-0.3447	-0.1233	C	7.0106	-0.5264	0.4227	H	6.2752	2.7260	-0.2924
C	-0.3724	0.2655	0.0505	C	5.7494	-1.0672	0.3682	H	8.2181	1.2627	0.2339
C	-0.5393	-2.4835	-0.4772	H	-5.9544	-3.0270	0.6096	H	7.8740	-1.1600	0.6505
C	-1.6630	-1.7234	-0.4965	H	-7.8619	-1.5281	0.0628	H	5.5908	-2.1413	0.5479

Table 3.500: Table of thermodynamic data as a function of temperature for Benzo[*c*]naphtho[1,2-*l*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.801	539.038	539.038	∞
100	124.332	374.572	866.067	-49.150	568.830	624.883	-326.399
200	245.858	495.951	650.673	-30.944	553.009	687.253	-179.488
250	316.461	558.342	625.937	-16.899	545.611	721.671	-150.782
298.15	385.298	619.981	619.981	0.000	539.038	756.192	-132.479
300	387.911	622.372	619.988	0.715	538.796	757.538	-131.896
350	456.635	687.382	624.965	21.846	532.756	794.487	-118.568
400	520.377	752.582	636.845	46.295	527.532	832.233	-108.676
450	578.122	817.268	653.305	73.783	523.031	870.596	-101.054
500	629.736	880.904	672.894	104.005	519.155	909.449	-95.008
600	716.289	1003.682	717.885	171.478	512.927	988.127	-86.022
700	784.766	1119.441	767.069	246.661	508.478	1067.710	-79.672
800	839.735	1227.949	817.972	327.982	505.592	1147.802	-74.942
900	884.587	1329.532	869.230	414.272	504.065	1228.167	-71.279
1000	921.691	1424.712	920.070	504.642	503.710	1308.652	-68.356
1100	952.717	1514.057	970.050	598.408	504.305	1389.135	-65.963
1200	978.884	1598.108	1018.921	695.024	505.689	1469.508	-63.965
1300	1001.109	1677.362	1066.551	794.053	507.659	1549.753	-62.269
1400	1020.103	1752.265	1112.880	895.138	510.068	1629.833	-60.809
1500	1036.428	1823.215	1157.892	997.985	512.823	1709.731	-59.537
1600	1050.532	1890.566	1201.597	1102.350	515.779	1789.427	-58.418
1700	1062.778	1954.630	1244.024	1208.030	518.853	1868.907	-57.423
1800	1073.462	2015.686	1285.212	1314.854	521.961	1948.277	-56.536
1900	1082.825	2073.982	1325.204	1422.678	525.067	2027.415	-55.736
2000	1091.066	2129.737	1364.047	1531.381	528.110	2106.420	-55.013
2100	1098.351	2183.150	1401.789	1640.860	531.004	2185.260	-54.354
2200	1104.815	2234.398	1438.478	1751.024	533.748	2263.969	-53.752
2300	1110.573	2283.638	1474.160	1861.799	536.334	2342.556	-53.200
2400	1115.720	2331.015	1508.882	1973.118	538.684	2420.981	-52.690
2500	1120.338	2376.656	1542.686	2084.925	540.811	2499.439	-52.222
2600	1124.494	2420.679	1575.613	2197.171	542.674	2577.688	-51.785
2700	1128.246	2463.189	1607.703	2309.811	544.279	2655.949	-51.381
2800	1131.643	2504.283	1638.994	2422.808	545.595	2734.181	-51.006
2900	1134.728	2544.048	1669.521	2536.129	546.590	2812.312	-50.654
3000	1137.537	2582.566	1699.317	2649.744	547.312	2890.443	-50.326
3100	1140.101	2619.908	1728.415	2763.628	547.676	2968.470	-50.017
3200	1142.448	2656.142	1756.843	2877.757	547.727	3046.572	-49.729
3300	1144.600	2691.330	1784.630	2992.111	547.445	3124.721	-49.459
3400	1146.579	2725.530	1811.803	3106.672	546.799	3202.788	-49.204
3500	1148.402	2758.793	1838.387	3221.422	545.795	3280.859	-48.963
3600	1150.084	2791.168	1864.405	3336.347	544.455	3359.060	-48.738
3700	1151.641	2822.701	1889.881	3451.435	542.746	3437.323	-48.525
3800	1153.083	2853.433	1914.835	3566.672	540.638	3515.568	-48.324
3900	1154.421	2883.402	1939.287	3682.048	538.177	3593.819	-48.133
4000	1155.666	2912.645	1963.257	3797.553	535.345	3672.291	-47.954
4100	1156.825	2941.196	1986.763	3913.178	532.101	3750.756	-47.784
4200	1157.906	2969.086	2009.820	4028.915	528.477	3829.295	-47.623
4300	1158.916	2996.344	2032.447	4144.757	524.457	3907.825	-47.470
4400	1159.861	3022.998	2054.658	4260.696	520.051	3986.556	-47.325
4500	1160.747	3049.073	2076.467	4376.727	515.275	4065.454	-47.190
4600	1161.577	3074.594	2097.889	4492.844	510.072	4144.470	-47.061
4700	1162.357	3099.584	2118.937	4609.041	504.457	4223.477	-46.938
4800	1163.091	3124.063	2139.623	4725.314	498.482	4302.725	-46.822
4900	1163.782	3148.053	2159.959	4841.658	492.066	4381.953	-46.711
5000	1164.433	3171.571	2179.957	4958.069	485.313	4461.523	-46.608

3.501. Benzo[*l*]naphtho[2,1-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-53-0
Point Group: C₁

Length: 18.01 Å
Width: 9.470 Å
Breadth: 5.055 Å
L/B Ratio: 1.902

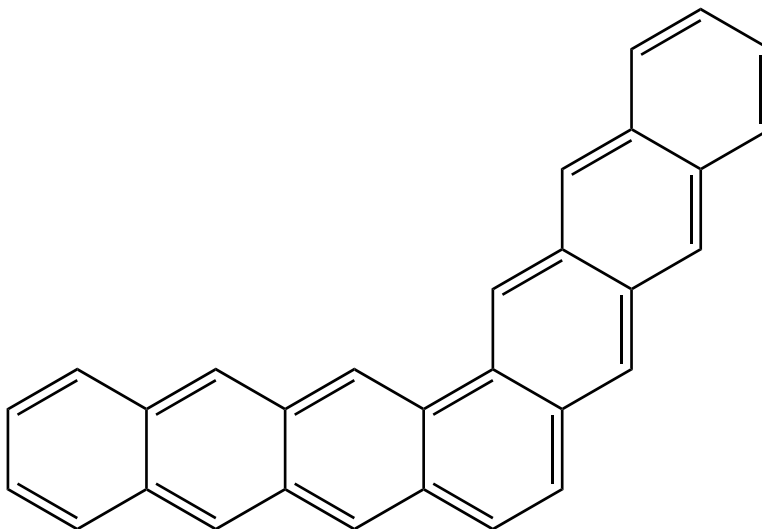
Cartesian coordinates:

C	6.8888	-1.7265	0.4098	C	-0.5342	-0.4561	-0.1548	H	3.5396	-2.3867	0.2777
C	6.8558	-0.3560	0.2608	C	-1.7465	0.2488	-0.1965	H	5.7327	-3.5512	0.5355
C	4.4844	-1.8217	0.2742	C	-1.7155	-2.5592	-0.2204	H	6.5370	2.2901	-0.0417
C	5.6961	-2.4635	0.4165	C	-0.5400	-1.8748	-0.1342	H	4.3783	3.4858	-0.3021
C	4.4284	-0.4228	0.1208	C	-2.9523	-1.8626	-0.2199	H	1.9451	3.4451	-0.4538
C	5.6253	0.3138	0.1144	C	-2.9907	-0.4645	-0.0886	H	1.9612	-1.5201	0.0870
C	5.5856	1.7457	-0.0415	C	-5.3655	-2.0177	-0.3422	H	-0.4906	3.4159	-0.6962
C	4.4104	2.3966	-0.1832	C	-4.1566	-2.6249	-0.3729	H	-2.6228	2.2145	-0.5935
C	3.1620	0.2701	-0.0304	C	-5.4566	-0.6209	-0.0381	H	-1.7217	-3.6541	-0.2765
C	3.1599	1.6793	-0.1827	C	-4.2870	0.1463	0.1491	H	0.4229	-2.4057	-0.0834
C	1.9502	2.3548	-0.3321	C	-4.4522	1.4618	0.6430	H	-6.2902	-2.5826	-0.5068
C	1.9515	-0.4194	-0.0287	C	-5.6989	2.0081	0.8393	H	-4.0722	-3.7056	-0.5367
C	0.7310	0.2504	-0.1693	C	-6.8547	1.2631	0.5562	H	-3.5676	2.0634	0.8923
C	0.7390	1.6551	-0.3279	C	-6.7329	-0.0387	0.1347	H	-5.7972	3.0286	1.2241
C	-0.5108	2.3375	-0.5002	H	7.8457	-2.2461	0.5235	H	-7.8414	1.7176	0.6906
C	-1.6842	1.6664	-0.4338	H	7.7859	0.2237	0.2550	H	-7.6250	-0.6461	-0.0576

Table 3.501: Table of thermodynamic data as a function of temperature for Benzo[*l*]naphtho[2,1-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.008	506.611	506.611	∞
100	125.532	376.953	869.636	-49.268	536.285	592.100	-309.275
200	246.435	498.980	653.847	-30.973	520.554	654.191	-170.854
250	316.746	561.467	629.093	-16.906	513.177	688.455	-143.842
298.15	385.329	623.135	623.135	0.000	506.611	722.825	-126.633
300	387.934	625.526	623.142	0.715	506.369	724.165	-126.086
350	456.436	690.523	628.119	21.841	500.325	760.956	-113.564
400	520.008	755.684	639.994	46.276	495.086	798.546	-104.277
450	577.637	820.319	656.447	73.743	490.564	836.755	-97.126
500	629.182	883.900	676.024	103.938	486.661	875.458	-91.457
600	715.703	1006.573	720.984	171.353	480.375	953.842	-83.038
700	784.228	1122.244	770.131	246.479	475.869	1033.139	-77.092
800	839.276	1230.686	820.997	327.751	472.934	1112.955	-72.667
900	884.212	1332.219	872.220	413.999	471.366	1193.049	-69.241
1000	921.391	1427.364	923.028	504.336	470.977	1273.267	-66.507
1100	952.481	1516.683	972.979	598.074	471.544	1353.486	-64.270
1200	978.699	1600.715	1021.824	694.670	472.908	1433.597	-62.402
1300	1000.965	1679.956	1069.431	793.683	474.862	1513.582	-60.815
1400	1019.992	1754.850	1115.739	894.755	477.258	1593.404	-59.449
1500	1036.342	1825.794	1160.733	997.592	480.003	1673.043	-58.259
1600	1050.466	1893.140	1204.421	1101.949	482.951	1752.482	-57.211
1700	1062.728	1957.200	1246.834	1207.623	486.019	1831.705	-56.280
1800	1073.424	2018.254	1288.008	1314.443	489.123	1910.817	-55.449
1900	1082.796	2076.547	1327.987	1422.264	492.226	1989.699	-54.700
2000	1091.045	2132.302	1366.819	1530.965	495.267	2068.447	-54.021
2100	1098.336	2185.714	1404.552	1640.441	498.159	2147.031	-53.403
2200	1104.804	2236.961	1441.232	1750.604	500.901	2225.484	-52.839
2300	1110.566	2286.201	1476.906	1861.378	503.486	2303.814	-52.320
2400	1115.716	2333.577	1511.620	1972.697	505.836	2381.984	-51.841
2500	1120.336	2379.218	1545.416	2084.504	507.963	2460.185	-51.402
2600	1124.494	2423.241	1578.337	2196.749	509.826	2538.178	-50.992
2700	1128.247	2465.751	1610.422	2309.389	511.430	2616.182	-50.612
2800	1131.646	2506.845	1641.707	2422.387	512.747	2694.159	-50.259
2900	1134.732	2546.611	1672.229	2535.708	513.742	2772.033	-49.929
3000	1137.541	2585.128	1702.020	2649.324	514.465	2849.907	-49.620
3100	1140.106	2622.470	1731.113	2763.208	514.829	2927.679	-49.330
3200	1142.453	2658.705	1759.537	2877.338	514.881	3005.524	-49.059
3300	1144.606	2693.893	1787.320	2991.692	514.599	3083.417	-48.805
3400	1146.585	2728.093	1814.489	3106.253	513.954	3161.228	-48.565
3500	1148.408	2761.356	1841.070	3221.004	512.950	3239.042	-48.339
3600	1150.090	2793.732	1867.085	3335.930	511.611	3316.987	-48.127
3700	1151.646	2825.265	1892.557	3451.018	509.903	3394.993	-47.928
3800	1153.088	2855.997	1917.508	3566.255	507.795	3472.983	-47.738
3900	1154.427	2885.966	1941.958	3681.632	505.335	3550.977	-47.559
4000	1155.672	2915.210	1965.925	3797.138	502.503	3629.192	-47.391
4100	1156.831	2943.761	1989.428	3912.763	499.260	3707.401	-47.232
4200	1157.912	2971.650	2012.484	4028.501	495.636	3785.683	-47.081
4300	1158.922	2998.909	2035.108	4144.343	491.617	3863.957	-46.937
4400	1159.867	3025.563	2057.316	4260.283	487.211	3942.432	-46.802
4500	1160.752	3051.638	2079.124	4376.315	482.436	4021.073	-46.674
4600	1161.583	3077.159	2100.544	4492.432	477.233	4099.832	-46.554
4700	1162.363	3102.149	2121.590	4608.630	471.619	4178.583	-46.439
4800	1163.096	3126.629	2142.274	4724.903	465.645	4257.575	-46.331
4900	1163.787	3150.618	2162.608	4841.247	459.230	4336.546	-46.227
5000	1164.438	3174.136	2182.604	4957.659	452.476	4415.860	-46.131

3.502. Heptaphene



Other names: Dibenzo[*b,n*]pentaphene
Anthra[2,3-*a*]naphthacene

Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 222-75-3
Point Group: C_{2v}

Length: 20.19 Å
Width: 10.36 Å
Breadth: 3.884 Å
L/B Ratio: 1.949

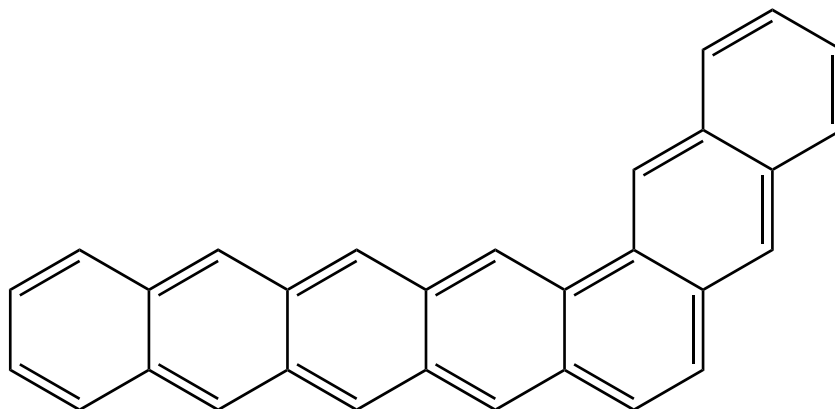
Cartesian coordinates:

C	7.1101	-2.6185	0.0000	C	-0.7313	0.9101	0.0000	H	7.6373	0.7641	0.0000
C	7.8022	-1.3710	0.0000	C	-1.4321	2.1642	0.0000	H	5.2113	-3.6088	0.0000
C	7.1145	-0.1990	0.0000	C	-2.8038	2.1886	0.0000	H	5.4898	1.9571	0.0000
C	5.7517	-2.6554	0.0000	C	-1.4434	-0.2629	0.0000	H	3.0624	-2.4179	0.0000
C	4.9892	-1.4402	0.0000	C	-2.8682	-0.2635	0.0000	H	3.3423	3.1454	0.0000
C	5.6798	-0.1952	0.0000	C	-3.5583	0.9791	0.0000	H	0.9073	-1.2251	0.0000
C	4.9584	0.9973	0.0000	C	-4.9590	0.9947	0.0000	H	1.2350	4.3412	0.0000
C	3.5955	-1.4592	0.0000	C	-3.5947	-1.4611	0.0000	H	-1.2373	4.3406	0.0000
C	2.8684	-0.2620	0.0000	C	-4.9884	-1.4428	0.0000	H	-3.3440	3.1436	0.0000
C	3.5577	0.9809	0.0000	C	-5.6797	-0.1982	0.0000	H	-0.9067	-1.2256	0.0000
C	2.8026	2.1901	0.0000	C	-7.1144	-0.2028	0.0000	H	-5.4908	1.9541	0.0000
C	1.4435	-0.2622	0.0000	C	-7.8015	-1.3752	0.0000	H	-3.0611	-2.4195	0.0000
C	0.7308	0.9105	0.0000	C	-7.1087	-2.6223	0.0000	H	-7.6377	0.7601	0.0000
C	1.4309	2.1650	0.0000	C	-5.7503	-2.6584	0.0000	H	-8.8963	-1.3839	0.0000
C	0.6709	3.4010	0.0000	H	7.6965	-3.5431	0.0000	H	-7.6947	-3.5472	0.0000
C	-0.6727	3.4006	0.0000	H	8.8971	-1.3792	0.0000	H	-5.2094	-3.6115	0.0000

Table 3.502: Table of thermodynamic data as a function of temperature for Heptaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-57.121	524.191	524.191	∞
100	125.329	368.641	863.354	-49.471	553.662	610.308	-318.785
200	247.523	490.965	646.596	-31.126	537.980	673.221	-175.824
250	318.339	553.752	621.719	-16.992	530.671	707.878	-147.900
298.15	387.250	615.730	615.730	0.000	524.191	742.612	-130.100
300	389.864	618.134	615.738	0.719	523.953	743.966	-129.533
350	458.512	683.441	620.739	21.946	518.009	781.119	-116.573
400	522.091	748.881	632.669	46.485	512.875	819.056	-106.956
450	579.649	813.758	649.194	74.054	508.455	857.599	-99.545
500	631.090	877.545	668.850	104.348	504.650	896.624	-93.668
600	717.395	1000.547	713.976	171.943	498.544	975.626	-84.934
700	785.745	1116.465	763.282	247.229	494.198	1055.513	-78.762
800	840.661	1225.100	814.294	328.645	491.408	1135.897	-74.165
900	885.491	1326.790	865.651	415.026	489.973	1216.541	-70.605
1000	922.582	1422.066	916.579	505.486	489.707	1297.295	-67.762
1100	953.591	1511.494	966.640	599.340	490.390	1378.039	-65.436
1200	979.735	1595.620	1015.585	696.043	491.860	1458.664	-63.493
1300	1001.931	1674.941	1063.283	795.156	493.914	1539.155	-61.843
1400	1020.891	1749.904	1109.675	896.321	496.404	1619.474	-60.422
1500	1037.178	1820.908	1154.744	999.245	499.236	1699.605	-59.184
1600	1051.244	1888.305	1198.504	1103.683	502.264	1779.529	-58.094
1700	1063.451	1952.412	1240.981	1209.432	505.407	1859.234	-57.126
1800	1074.097	2013.505	1282.215	1316.321	508.581	1938.823	-56.262
1900	1083.424	2071.834	1322.251	1424.207	511.749	2018.178	-55.482
2000	1091.630	2127.619	1361.135	1532.968	514.850	2097.396	-54.777
2100	1098.881	2181.059	1398.915	1642.501	517.799	2176.446	-54.135
2200	1105.314	2232.330	1435.641	1752.717	520.594	2255.364	-53.548
2300	1111.043	2281.592	1471.357	1863.541	523.228	2334.156	-53.009
2400	1116.163	2328.988	1506.111	1974.906	525.624	2412.785	-52.512
2500	1120.755	2374.647	1539.945	2086.756	527.794	2491.445	-52.055
2600	1124.887	2418.686	1572.900	2199.041	529.698	2569.893	-51.629
2700	1128.617	2461.210	1605.018	2311.720	531.341	2648.353	-51.234
2800	1131.994	2502.317	1636.334	2424.753	532.693	2726.783	-50.868
2900	1135.061	2542.095	1666.885	2538.108	533.722	2805.109	-50.524
3000	1137.852	2580.623	1696.704	2651.756	534.477	2883.435	-50.204
3100	1140.400	2617.975	1725.823	2765.671	534.871	2961.656	-49.903
3200	1142.731	2654.219	1754.272	2879.829	534.952	3039.951	-49.621
3300	1144.869	2689.416	1782.079	2994.210	534.697	3118.291	-49.357
3400	1146.835	2723.623	1809.271	3108.797	534.078	3196.550	-49.108
3500	1148.645	2756.893	1835.873	3223.572	533.098	3274.811	-48.873
3600	1150.316	2789.276	1861.908	3338.521	531.782	3353.201	-48.653
3700	1151.862	2820.814	1887.401	3453.631	530.096	3431.653	-48.445
3800	1153.294	2851.552	1912.370	3568.890	528.010	3510.087	-48.249
3900	1154.623	2881.527	1936.838	3684.287	525.569	3588.526	-48.062
4000	1155.858	2910.775	1960.822	3799.811	522.756	3667.185	-47.888
4100	1157.009	2939.330	1984.341	3915.455	519.531	3745.836	-47.722
4200	1158.083	2967.224	2007.412	4031.211	515.925	3824.562	-47.564
4300	1159.086	2994.487	2030.052	4147.070	511.922	3903.278	-47.414
4400	1160.024	3021.144	2052.275	4263.026	507.533	3982.195	-47.274
4500	1160.903	3047.223	2074.096	4379.072	502.773	4061.278	-47.141
4600	1161.727	3072.748	2095.529	4495.204	497.585	4140.478	-47.016
4700	1162.501	3097.740	2116.588	4611.416	491.985	4219.670	-46.895
4800	1163.230	3122.223	2137.285	4727.703	486.025	4299.103	-46.783
4900	1163.915	3146.215	2157.631	4844.061	479.622	4378.514	-46.675
5000	1164.561	3169.736	2177.639	4960.485	472.882	4458.268	-46.574

3.503. Benzo[*p*]hexaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 222-81-1
Point Group: C_s

Length: 20.32 Å
Width: 10.25 Å
Breadth: 3.885 Å
L/B Ratio: 1.983

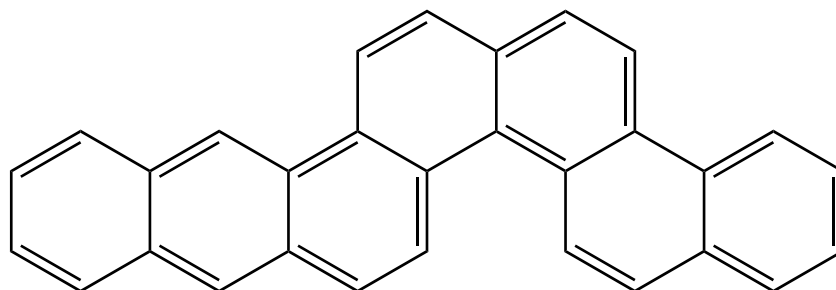
Cartesian coordinates:

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C	8.1489	-0.4521	0.0000	C	-1.2419	2.0879	0.0000	H	6.1735	-3.2520	0.0000
C	7.2037	0.5190	0.0000	C	-2.2792	3.1022	0.0000	H	5.1091	2.2209	0.0000
C	6.4694	-2.1968	0.0000	C	-3.5827	2.7754	0.0000	H	3.8027	-2.6114	0.0000
C	5.4298	-1.2003	0.0000	C	-3.0414	0.3504	0.0000	H	2.7431	2.8603	0.0000
C	5.8036	0.1822	0.0000	C	-4.0168	1.3915	0.0000	H	1.4367	-1.9713	0.0000
C	4.8274	1.1606	0.0000	C	-5.3619	1.0809	0.0000	H	0.3745	3.4989	0.0000
C	4.0936	-1.5536	0.0000	C	-3.4545	-0.9673	0.0000	H	-0.9409	-1.3321	0.0000
C	3.0842	-0.5625	0.0000	C	-4.8279	-1.2991	0.0000	H	-1.9604	4.1513	0.0000
C	3.4561	0.8132	0.0000	C	-5.7905	-0.2661	0.0000	H	-4.3592	3.5494	0.0000
C	2.4541	1.8020	0.0000	C	-7.1737	-0.6045	0.0000	H	-6.1146	1.8791	0.0000
C	1.7204	-0.9116	0.0000	C	-7.5626	-1.9145	0.0000	H	-2.7004	-1.7710	0.0000
C	0.7378	0.0700	0.0000	C	-6.5964	-2.9512	0.0000	H	-7.9145	0.2031	0.0000
C	1.1106	1.4495	0.0000	C	-5.2623	-2.6552	0.0000	H	-8.6248	-2.1804	0.0000
C	0.0798	2.4420	0.0000	H	8.5689	-2.5884	0.0000	H	-6.9362	-3.9921	0.0000
C	-0.6518	-0.2685	0.0000	H	9.2145	-0.2007	0.0000	H	-4.5087	-3.4507	0.0000

Table 3.503: Table of thermodynamic data as a function of temperature for Benzo[*p*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.143	529.620	529.620	∞
100	125.328	376.120	870.688	-49.457	559.105	615.003	-321.238
200	247.459	498.404	653.993	-31.118	543.418	677.171	-176.855
250	318.259	561.175	629.122	-16.987	536.105	711.456	-148.648
298.15	387.117	623.136	623.136	0.000	529.620	745.833	-130.664
300	389.727	625.539	623.143	0.719	529.381	747.173	-130.092
350	458.306	690.820	628.142	21.937	523.429	783.957	-116.997
400	521.826	756.228	640.068	46.464	518.283	821.525	-107.278
450	579.341	821.071	656.585	74.019	513.849	859.702	-99.790
500	630.757	884.825	676.232	104.296	510.028	898.362	-93.849
600	717.049	1007.763	721.335	171.857	503.888	976.640	-85.022
700	785.414	1123.630	770.617	247.109	499.508	1055.808	-78.784
800	840.355	1232.222	821.605	328.494	496.686	1135.478	-74.138
900	885.214	1333.878	872.938	414.845	495.221	1215.411	-70.539
1000	922.331	1429.125	923.846	505.279	494.929	1295.458	-67.666
1100	953.365	1518.531	973.886	599.109	495.588	1375.497	-65.316
1200	979.531	1602.638	1022.813	695.790	497.037	1455.419	-63.351
1300	1001.746	1681.943	1070.494	794.884	499.072	1535.209	-61.684
1400	1020.723	1756.893	1116.871	896.032	501.544	1614.829	-60.249
1500	1037.026	1827.886	1161.926	998.940	504.359	1694.261	-58.998
1600	1051.105	1895.274	1205.673	1103.363	507.374	1773.488	-57.897
1700	1063.325	1959.373	1248.138	1209.099	510.504	1852.496	-56.919
1800	1073.981	2020.459	1289.361	1315.976	513.665	1931.390	-56.046
1900	1083.317	2078.782	1329.387	1423.851	516.822	2010.049	-55.259
2000	1091.532	2134.562	1368.261	1532.602	519.913	2088.573	-54.547
2100	1098.791	2187.997	1406.033	1642.126	522.852	2166.929	-53.898
2200	1105.231	2239.265	1442.750	1752.333	525.639	2245.153	-53.306
2300	1110.965	2288.523	1478.459	1863.148	528.265	2323.252	-52.762
2400	1116.091	2335.916	1513.205	1974.506	530.654	2401.188	-52.259
2500	1120.688	2381.571	1547.032	2086.349	532.817	2479.155	-51.798
2600	1124.825	2425.608	1579.981	2198.628	534.714	2556.912	-51.368
2700	1128.559	2468.130	1612.093	2311.300	536.350	2634.679	-50.970
2800	1131.939	2509.235	1643.404	2424.328	537.697	2712.417	-50.600
2900	1135.009	2549.011	1673.950	2537.678	538.721	2790.052	-50.253
3000	1137.803	2587.537	1703.764	2651.321	539.470	2867.686	-49.930
3100	1140.354	2624.888	1732.878	2765.230	539.860	2945.216	-49.626
3200	1142.688	2661.130	1761.322	2879.384	539.936	3022.819	-49.341
3300	1144.829	2696.326	1789.125	2993.762	539.677	3100.469	-49.075
3400	1146.796	2730.532	1816.313	3108.344	539.054	3178.036	-48.824
3500	1148.609	2763.801	1842.911	3223.116	538.070	3255.607	-48.586
3600	1150.282	2796.182	1868.943	3338.061	536.751	3333.306	-48.364
3700	1151.829	2827.720	1894.431	3453.168	535.062	3411.068	-48.155
3800	1153.262	2858.457	1919.398	3568.423	532.972	3488.811	-47.956
3900	1154.593	2888.431	1943.862	3683.817	530.529	3566.559	-47.768
4000	1155.830	2917.678	1967.843	3799.339	527.712	3644.528	-47.592
4100	1156.982	2946.233	1991.360	3914.980	524.485	3722.489	-47.424
4200	1158.057	2974.126	2014.428	4030.733	520.876	3800.525	-47.265
4300	1159.061	3001.388	2037.065	4146.589	516.871	3878.551	-47.114
4400	1160.000	3028.045	2059.285	4262.543	512.479	3956.777	-46.972
4500	1160.880	3054.124	2081.104	4378.587	507.717	4035.170	-46.838
4600	1161.705	3079.648	2102.535	4494.717	502.527	4113.680	-46.711
4700	1162.480	3104.640	2123.592	4610.926	496.924	4192.183	-46.590
4800	1163.209	3129.122	2144.286	4727.211	490.962	4270.925	-46.476
4900	1163.896	3153.113	2164.630	4843.567	484.558	4349.646	-46.367
5000	1164.543	3176.634	2184.636	4959.989	477.815	4428.711	-46.265

3.504. Benzo[*b*]naphtho[1,2-*l*]chrysene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-90-5
Point Group: C_1

Length: 19.18 Å
Width: 9.386 Å
Breadth: 4.971 Å
L/B Ratio: 2.043

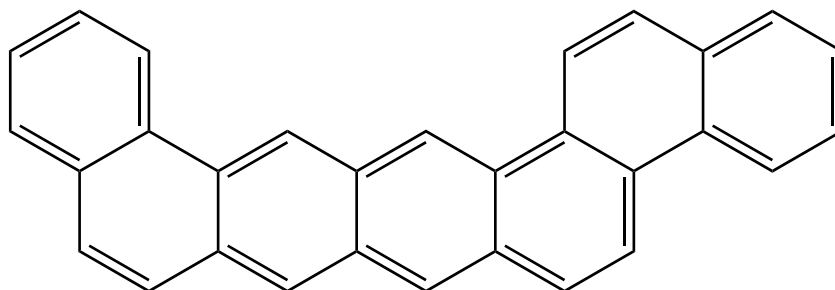
Cartesian coordinates:

C	7.5033	-0.4474	0.4005	C	-1.1369	-2.1138	-0.0534	H	6.5341	2.7461	-0.3527
C	7.5954	0.9433	0.1177	C	-1.0914	-0.7071	-0.0424	H	6.2118	-2.1414	0.6417
C	6.4733	1.6740	-0.1340	C	-3.5464	-2.1116	-0.2340	H	4.0856	2.8534	-0.5978
C	6.2919	-1.0703	0.4245	C	-2.3796	-2.8033	-0.1740	H	3.7678	-2.0332	0.4031
C	5.0943	-0.3336	0.1654	C	-3.5551	-0.6964	-0.0623	H	1.6638	2.9401	-0.9295
C	5.1865	1.0517	-0.1173	C	-2.3470	-0.0036	0.0984	H	-0.5405	1.8816	-0.7810
C	4.0163	1.7814	-0.3757	C	-2.4178	1.3733	0.4885	H	-0.0196	-3.9745	0.0866
C	3.8367	-0.9552	0.1869	C	-3.5990	2.0344	0.5939	H	2.1923	-2.8451	0.2464
C	2.6747	-0.2319	-0.0610	C	-4.8154	0.0035	-0.0044	H	-4.5076	-2.6278	-0.3788
C	2.7753	1.1561	-0.3507	C	-4.8326	1.3730	0.3110	H	-2.3714	-3.8978	-0.2345
C	1.5713	1.8894	-0.6303	C	-6.0619	2.0716	0.3608	H	-1.4863	1.9028	0.7309
C	0.3590	1.2988	-0.5399	C	-7.2406	1.4157	0.1042	H	-3.6278	3.0848	0.9060
C	1.3625	-0.8540	-0.0273	C	-7.2314	0.0422	-0.2055	H	-6.0574	3.1400	0.6046
C	0.2018	-0.0852	-0.1718	C	-6.0464	-0.6496	-0.2563	H	-8.1942	1.9526	0.1389
C	0.0551	-2.8815	0.0485	H	8.4237	-1.0066	0.5982	H	-8.1788	-0.4692	-0.4049
C	1.2666	-2.2642	0.1156	H	8.5837	1.4143	0.1064	H	-6.0332	-1.7242	-0.4931

Table 3.504: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[1,2-*l*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.030	515.804	515.804	∞
100	125.395	376.050	869.162	-49.311	545.434	601.340	-314.101
200	246.679	498.112	653.158	-31.009	529.710	663.522	-173.290
250	317.120	560.669	628.375	-16.926	522.349	697.827	-145.800
298.15	385.779	622.409	622.409	0.000	515.804	732.234	-128.282
300	388.385	624.804	622.417	0.716	515.563	733.575	-127.724
350	456.918	689.873	627.399	21.866	509.541	770.401	-114.974
400	520.490	755.099	639.287	46.325	504.327	808.021	-105.515
450	578.100	819.790	655.757	73.815	499.828	846.258	-98.229
500	629.618	883.418	675.352	104.033	495.948	884.986	-92.452
600	716.077	1006.165	720.350	171.489	489.703	963.414	-83.871
700	784.543	1121.889	769.534	246.649	485.231	1042.750	-77.809
800	839.542	1230.370	820.433	327.950	482.325	1122.599	-73.297
900	884.436	1331.931	871.685	414.222	480.781	1202.723	-69.803
1000	921.582	1427.098	922.519	504.579	480.413	1282.968	-67.014
1100	952.644	1516.434	972.493	598.336	480.998	1363.213	-64.732
1200	978.841	1600.480	1021.358	694.946	482.377	1443.349	-62.826
1300	1001.089	1679.731	1068.983	793.972	484.344	1523.357	-61.208
1400	1020.100	1754.634	1115.308	895.056	486.752	1603.200	-59.815
1500	1036.438	1825.585	1160.316	997.903	489.507	1682.861	-58.601
1600	1050.551	1892.936	1204.018	1102.270	492.464	1762.320	-57.533
1700	1062.804	1957.002	1246.442	1207.952	495.540	1841.563	-56.583
1800	1073.492	2018.059	1287.627	1314.778	498.651	1920.696	-55.736
1900	1082.858	2076.356	1327.616	1422.606	501.761	1999.596	-54.972
2000	1091.101	2132.114	1366.457	1531.313	504.807	2078.364	-54.280
2100	1098.387	2185.529	1404.198	1640.795	507.705	2156.966	-53.650
2200	1104.851	2236.778	1440.886	1750.963	510.452	2235.438	-53.075
2300	1110.609	2286.020	1476.567	1861.741	513.042	2313.786	-52.547
2400	1115.756	2333.398	1511.288	1973.064	515.396	2391.973	-52.059
2500	1120.373	2379.040	1545.090	2084.875	517.526	2470.193	-51.611
2600	1124.528	2423.064	1578.017	2197.123	519.393	2548.203	-51.193
2700	1128.279	2465.576	1610.107	2309.767	521.000	2626.225	-50.806
2800	1131.675	2506.671	1641.397	2422.767	522.320	2704.219	-50.447
2900	1134.759	2546.438	1671.924	2536.091	523.318	2782.111	-50.110
3000	1137.567	2584.956	1701.719	2649.710	524.043	2860.002	-49.796
3100	1140.130	2622.299	1730.816	2763.597	524.410	2937.791	-49.500
3200	1142.476	2658.534	1759.244	2877.729	524.464	3015.654	-49.224
3300	1144.627	2693.724	1787.031	2992.085	524.185	3093.563	-48.966
3400	1146.605	2727.924	1814.204	3106.648	523.542	3171.391	-48.721
3500	1148.427	2761.188	1840.787	3221.401	522.540	3249.222	-48.491
3600	1150.108	2793.564	1866.806	3336.329	521.203	3327.183	-48.275
3700	1151.664	2825.097	1892.281	3451.419	519.496	3405.207	-48.072
3800	1153.105	2855.829	1917.235	3566.658	517.391	3483.213	-47.879
3900	1154.442	2885.799	1941.688	3682.036	514.932	3561.224	-47.696
4000	1155.686	2915.043	1965.657	3797.543	512.101	3639.456	-47.525
4100	1156.845	2943.594	1989.163	3913.171	508.859	3717.681	-47.363
4200	1157.925	2971.485	2012.221	4028.910	505.237	3795.980	-47.209
4300	1158.935	2998.743	2034.847	4144.753	501.219	3874.271	-47.062
4400	1159.879	3025.398	2057.058	4260.694	496.815	3952.762	-46.924
4500	1160.764	3051.473	2078.867	4376.727	492.041	4031.420	-46.795
4600	1161.594	3076.995	2100.289	4492.845	486.839	4110.195	-46.672
4700	1162.373	3101.985	2121.337	4609.044	481.226	4188.963	-46.554
4800	1163.106	3126.464	2142.023	4725.318	475.253	4267.971	-46.444
4900	1163.797	3150.454	2162.359	4841.664	468.838	4346.958	-46.338
5000	1164.447	3173.972	2182.357	4958.076	462.086	4426.289	-46.240

3.505. Benzo[*a*]naphtho[1,2-*l*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 112498-96-1
Point Group: C_s

Length: 19.08 Å
Width: 9.514 Å
Breadth: 3.885 Å
L/B Ratio: 2.005

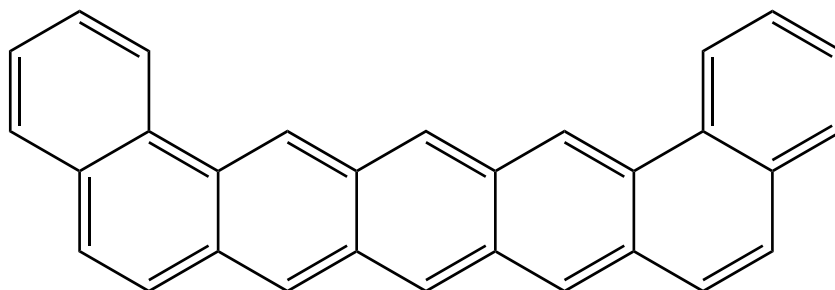
Cartesian coordinates:

C	7.1100	-2.2222	0.0000	C	-1.3511	0.3509	0.0000	H	3.7226	-2.6514	0.0000
C	7.1624	-0.8416	0.0000	C	-1.2543	1.7758	0.0000	H	5.8401	-3.9725	0.0000
C	4.7017	-2.1482	0.0000	C	-2.4632	2.5602	0.0000	H	7.0155	1.8336	0.0000
C	5.8741	-2.8782	0.0000	C	-3.6763	1.9663	0.0000	H	4.9399	3.1888	0.0000
C	4.7341	-0.7430	0.0000	C	-2.6669	-0.2639	0.0000	H	2.5122	3.3275	0.0000
C	5.9766	-0.0870	0.0000	C	-3.8080	0.5326	0.0000	H	2.2013	-1.6656	0.0000
C	6.0284	1.3567	0.0000	C	-4.0232	-2.2766	0.0000	H	0.0602	3.4838	0.0000
C	4.8996	2.0932	0.0000	C	-2.7980	-1.6840	0.0000	H	-0.2646	-1.5066	0.0000
C	3.5059	0.0389	0.0000	C	-5.2093	-1.4846	0.0000	H	-2.3695	3.6524	0.0000
C	3.5956	1.4676	0.0000	C	-5.1077	-0.0800	0.0000	H	-4.6030	2.5606	0.0000
C	2.4478	2.2323	0.0000	C	-6.2987	0.6900	0.0000	H	-4.1192	-3.3684	0.0000
C	2.2663	-0.5655	0.0000	C	-7.5268	0.0808	0.0000	H	-1.8767	-2.2868	0.0000
C	1.0781	0.2050	0.0000	C	-7.6237	-1.3263	0.0000	H	-6.2110	1.7871	0.0000
C	1.1698	1.6208	0.0000	C	-6.4885	-2.0954	0.0000	H	-8.4428	0.6806	0.0000
C	-0.0128	2.3891	0.0000	H	8.0350	-2.8080	0.0000	H	-8.6131	-1.7952	0.0000
C	-0.1918	-0.4072	0.0000	H	8.1290	-0.3250	0.0000	H	-6.5540	-3.1894	0.0000

Table 3.505: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[1,2-*l*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.361	495.993	495.993	∞
100	126.951	380.771	875.583	-49.481	525.454	580.887	-303.418
200	247.447	503.608	658.967	-31.072	509.838	642.550	-167.813
250	317.750	566.320	634.138	-16.954	502.511	676.576	-141.360
298.15	386.315	628.163	628.163	0.000	495.993	710.708	-124.511
300	388.918	630.561	628.171	0.717	495.754	712.039	-123.974
350	457.362	695.705	633.159	21.891	489.757	748.574	-111.716
400	520.852	760.985	645.060	46.370	484.562	785.902	-102.626
450	578.393	825.715	661.544	73.877	480.080	823.844	-95.627
500	629.855	889.370	681.155	104.108	476.213	862.274	-90.079
600	716.242	1012.153	726.181	171.583	469.988	940.105	-81.842
700	784.675	1127.901	775.389	246.758	465.531	1018.841	-76.025
800	839.661	1236.398	826.308	328.071	462.637	1098.088	-71.696
900	884.553	1337.973	877.579	414.355	461.105	1177.609	-68.345
1000	921.699	1433.153	928.428	504.724	460.748	1257.249	-65.671
1100	952.762	1522.500	978.416	598.493	461.345	1336.888	-63.482
1200	978.958	1606.556	1027.293	695.115	462.735	1416.417	-61.654
1300	1001.204	1685.816	1074.930	794.153	464.714	1495.817	-60.101
1400	1020.212	1760.727	1121.264	895.248	467.133	1575.051	-58.765
1500	1036.546	1831.686	1166.281	998.106	469.900	1654.102	-57.600
1600	1050.655	1899.044	1209.992	1102.483	472.867	1732.951	-56.574
1700	1062.903	1963.116	1252.424	1208.175	475.953	1811.583	-55.662
1800	1073.586	2024.179	1293.617	1315.011	479.074	1890.103	-54.848
1900	1082.947	2082.481	1333.613	1422.848	482.193	1968.392	-54.114
2000	1091.186	2138.243	1372.461	1531.564	485.248	2046.547	-53.449
2100	1098.466	2191.661	1410.207	1641.054	488.154	2124.536	-52.844
2200	1104.926	2242.914	1446.901	1751.229	490.909	2202.394	-52.290
2300	1110.680	2292.159	1482.588	1862.015	493.506	2280.128	-51.782
2400	1115.823	2339.540	1517.313	1973.345	495.867	2357.702	-51.313
2500	1120.436	2385.186	1551.121	2085.162	498.004	2435.307	-50.882
2600	1124.588	2429.212	1584.052	2197.417	499.876	2512.702	-50.480
2700	1128.336	2471.726	1616.146	2310.066	501.490	2590.110	-50.108
2800	1131.729	2512.823	1647.440	2423.072	502.815	2667.489	-49.762
2900	1134.810	2552.592	1677.970	2536.402	503.818	2744.765	-49.438
3000	1137.616	2591.112	1707.770	2650.025	504.549	2822.041	-49.135
3100	1140.176	2628.456	1736.870	2763.917	504.920	2899.214	-48.850
3200	1142.519	2664.693	1765.301	2878.053	504.979	2976.461	-48.585
3300	1144.669	2699.883	1793.091	2992.414	504.704	3053.754	-48.336
3400	1146.644	2734.085	1820.267	3106.981	504.065	3130.966	-48.100
3500	1148.464	2767.350	1846.853	3221.738	503.066	3208.182	-47.879
3600	1150.144	2799.727	1872.874	3336.669	501.733	3285.526	-47.671
3700	1151.698	2831.261	1898.352	3451.762	500.030	3362.934	-47.475
3800	1153.137	2861.994	1923.309	3567.005	497.927	3440.323	-47.290
3900	1154.474	2891.965	1947.763	3682.386	495.472	3517.718	-47.114
4000	1155.716	2921.210	1971.736	3797.897	492.644	3595.333	-46.949
4100	1156.873	2949.762	1995.243	3913.527	489.405	3672.941	-46.793
4200	1157.953	2977.653	2018.303	4029.269	485.786	3750.624	-46.645
4300	1158.961	3004.912	2040.932	4145.115	481.770	3828.298	-46.504
4400	1159.904	3031.567	2063.144	4261.059	477.369	3906.172	-46.371
4500	1160.788	3057.643	2084.956	4377.094	472.597	3984.212	-46.247
4600	1161.617	3083.165	2106.379	4493.215	467.398	4062.371	-46.129
4700	1162.396	3108.155	2127.429	4609.416	461.787	4140.522	-46.016
4800	1163.128	3132.636	2148.116	4725.692	455.817	4218.913	-45.910
4900	1163.817	3156.626	2168.454	4842.040	449.404	4297.283	-45.809
5000	1164.467	3180.145	2188.454	4958.454	442.654	4375.996	-45.715

3.506. Dibenzo[*a,n*]pentacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 227-07-6
Point Group: C_{2v}

Length: 19.12 Å
Width: 9.503 Å
Breadth: 3.884 Å
L/B Ratio: 2.012

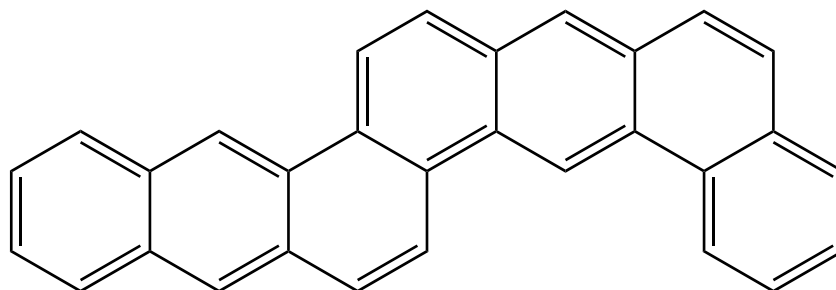
Cartesian coordinates:

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C	-4.9903	2.1239	0.0000	C	2.4609	-2.1023	0.0000	H	-7.0399	-1.9998	0.0000
C	-6.2088	2.7761	0.0000	C	2.4592	0.7038	0.0000	H	-4.8825	-3.2189	0.0000
C	-4.9307	0.7205	0.0000	C	3.6518	0.0229	0.0000	H	-2.4521	-3.2007	0.0000
C	-6.1276	-0.0154	0.0000	C	3.6495	-1.4145	0.0000	H	-2.4642	1.8048	0.0000
C	-6.0853	-1.4609	0.0000	C	4.9136	-2.1207	0.0000	H	0.0008	-3.2021	0.0000
C	-4.9126	-2.1230	0.0000	C	6.0860	-1.4581	0.0000	H	-0.0004	1.8025	0.0000
C	-3.6518	0.0212	0.0000	C	4.9303	0.7228	0.0000	H	2.4536	-3.1995	0.0000
C	-3.6489	-1.4162	0.0000	C	6.1277	-0.0125	0.0000	H	2.4635	1.8060	0.0000
C	-2.4598	-2.1035	0.0000	C	7.3592	0.6626	0.0000	H	4.8841	-3.2167	0.0000
C	-2.4595	0.7027	0.0000	C	7.3971	2.0447	0.0000	H	7.0409	-1.9964	0.0000
C	-1.2141	0.0124	0.0000	C	6.2074	2.7790	0.0000	H	8.2904	0.0846	0.0000
C	-1.2140	-1.4126	0.0000	C	4.9892	2.1261	0.0000	H	8.3586	2.5683	0.0000
C	0.0005	-2.1050	0.0000	H	-8.3599	2.5643	0.0000	H	6.2437	3.8733	0.0000
C	-0.0001	0.7056	0.0000	H	-8.2904	0.0806	0.0000	H	4.0451	2.6924	0.0000

Table 3.506: Table of thermodynamic data as a function of temperature for Dibenzo[*a,n*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-57.068	513.211	513.211	∞
100	125.716	371.229	864.479	-49.325	542.828	599.215	-312.992
200	246.744	493.394	648.441	-31.010	527.118	661.872	-172.860
250	317.133	555.960	623.659	-16.925	519.758	696.413	-145.505
298.15	385.685	617.695	617.695	0.000	513.211	731.047	-128.074
300	388.287	620.088	617.702	0.716	512.970	732.397	-127.519
350	456.679	685.132	622.683	21.857	506.940	769.459	-114.833
400	520.121	750.317	634.565	46.301	501.711	807.318	-105.423
450	577.635	814.959	651.025	73.770	497.191	845.795	-98.175
500	629.097	878.534	670.608	103.963	493.286	884.766	-92.429
600	715.541	1001.183	715.575	171.365	486.987	963.687	-83.895
700	784.072	1116.829	764.723	246.475	482.465	1043.525	-77.867
800	839.165	1225.253	815.587	327.733	479.516	1123.883	-73.381
900	884.155	1326.776	866.807	413.972	477.939	1204.521	-69.907
1000	921.385	1421.918	917.612	504.306	477.547	1285.283	-67.135
1100	952.516	1511.238	967.560	598.046	478.116	1366.047	-64.867
1200	978.766	1595.275	1016.403	694.647	479.485	1446.703	-62.972
1300	1001.055	1674.522	1064.009	793.667	481.447	1527.232	-61.364
1400	1020.097	1749.423	1110.316	894.750	483.853	1607.596	-59.979
1500	1036.456	1820.374	1155.309	997.598	486.609	1687.778	-58.772
1600	1050.585	1887.728	1198.999	1101.967	489.569	1767.758	-57.710
1700	1062.849	1951.796	1241.412	1207.652	492.649	1847.522	-56.766
1800	1073.545	2012.856	1282.587	1314.484	495.764	1927.174	-55.924
1900	1082.916	2071.156	1322.568	1422.317	498.879	2006.596	-55.164
2000	1091.162	2126.917	1361.402	1531.030	501.932	2085.883	-54.477
2100	1098.449	2180.335	1399.136	1640.518	504.836	2165.004	-53.850
2200	1104.913	2231.587	1435.817	1750.692	507.589	2243.995	-53.278
2300	1110.671	2280.831	1471.494	1861.477	510.185	2322.863	-52.753
2400	1115.817	2328.212	1506.209	1972.806	512.545	2401.569	-52.268
2500	1120.432	2373.857	1540.008	2084.623	514.682	2480.307	-51.822
2600	1124.586	2417.883	1572.931	2196.877	516.554	2558.835	-51.407
2700	1128.335	2460.397	1605.017	2309.526	518.167	2637.375	-51.022
2800	1131.730	2501.494	1636.304	2422.532	519.492	2715.887	-50.664
2900	1134.812	2541.263	1666.828	2535.862	520.496	2794.296	-50.330
3000	1137.618	2579.783	1696.621	2649.485	521.227	2872.705	-50.017
3100	1140.179	2617.127	1725.715	2763.377	521.598	2951.011	-49.723
3200	1142.523	2653.364	1754.141	2877.514	521.657	3029.391	-49.449
3300	1144.673	2688.555	1781.926	2991.875	521.383	3107.817	-49.192
3400	1146.648	2722.757	1809.097	3106.443	520.744	3186.162	-48.948
3500	1148.469	2756.022	1835.679	3221.200	519.746	3264.510	-48.719
3600	1150.149	2788.399	1861.696	3336.132	518.413	3342.988	-48.504
3700	1151.702	2819.933	1887.170	3451.225	516.711	3421.528	-48.302
3800	1153.142	2850.667	1912.122	3566.469	514.609	3500.050	-48.111
3900	1154.478	2880.637	1936.573	3681.850	512.153	3578.577	-47.929
4000	1155.721	2909.882	1960.542	3797.361	509.326	3657.326	-47.759
4100	1156.878	2938.434	1984.046	3912.992	506.088	3736.067	-47.597
4200	1157.957	2966.325	2007.103	4028.734	502.469	3814.882	-47.444
4300	1158.966	2993.585	2029.729	4144.581	498.454	3893.688	-47.298
4400	1159.909	3020.240	2051.938	4260.525	494.053	3972.695	-47.161
4500	1160.792	3046.316	2073.747	4376.561	489.282	4051.869	-47.032
4600	1161.621	3071.838	2095.168	4492.682	484.083	4131.160	-46.910
4700	1162.400	3096.829	2116.215	4608.883	478.472	4210.443	-46.793
4800	1163.132	3121.309	2136.901	4725.160	472.502	4289.967	-46.683
4900	1163.822	3145.299	2157.236	4841.508	466.090	4369.469	-46.578
5000	1164.471	3168.818	2177.233	4957.923	459.340	4449.315	-46.481

3.507. Benzo[*b*]naphtho[2,1-*k*]chrysene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 115747-91-6
Point Group: C_s

Length: 19.06 Å
Width: 9.520 Å
Breadth: 3.886 Å
L/B Ratio: 2.002

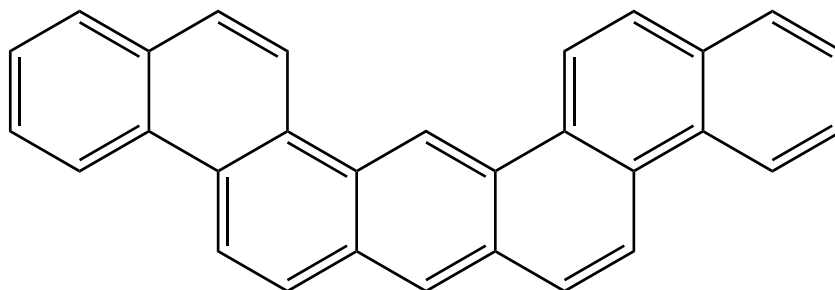
Cartesian coordinates:

C	-6.8898	2.1862	0.0000	C	0.3666	0.1069	0.0000	H	-3.4867	2.4829	0.0000
C	-6.9972	0.8108	0.0000	C	1.4783	-0.7268	0.0000	H	-5.5517	3.8863	0.0000
C	-4.4857	2.0202	0.0000	C	1.7803	2.0844	0.0000	H	-6.9513	-1.8706	0.0000
C	-5.6271	2.7941	0.0000	C	0.5452	1.5320	0.0000	H	-4.9247	-3.3019	0.0000
C	-4.5734	0.6151	0.0000	C	2.9566	1.2576	0.0000	H	-2.4989	-3.5272	0.0000
C	-5.8407	0.0079	0.0000	C	2.8107	-0.1578	0.0000	H	-2.0002	1.4438	0.0000
C	-5.9476	-1.4298	0.0000	C	3.9500	-0.9581	0.0000	H	-0.0729	-3.7869	0.0000
C	-4.8447	-2.2087	0.0000	C	4.2261	1.8283	0.0000	H	2.2014	-2.7776	0.0000
C	-3.3819	-0.2152	0.0000	C	5.3716	1.0207	0.0000	H	1.9116	3.1726	0.0000
C	-3.5241	-1.6280	0.0000	C	5.2309	-0.3901	0.0000	H	-0.3601	2.1587	0.0000
C	-2.3916	-2.4352	0.0000	C	6.4064	-1.2051	0.0000	H	3.8370	-2.0541	0.0000
C	-2.1086	0.3422	0.0000	C	7.6422	-0.6328	0.0000	H	4.3349	2.9200	0.0000
C	-0.9598	-0.4617	0.0000	C	7.7832	0.7831	0.0000	H	6.2882	-2.2946	0.0000
C	-1.1086	-1.8691	0.0000	C	6.6846	1.5879	0.0000	H	8.5454	-1.2517	0.0000
C	0.0593	-2.6989	0.0000	H	-7.7901	2.8094	0.0000	H	8.7908	1.2117	0.0000
C	1.2988	-2.1472	0.0000	H	-7.9830	0.3319	0.0000	H	6.7834	2.6793	0.0000

Table 3.507: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[2,1-*k*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.583	492.088	492.088	∞
100	127.660	384.498	880.552	-49.605	521.424	576.485	-301.119
200	248.055	507.807	663.450	-31.129	505.875	637.747	-166.559
250	318.324	570.650	638.578	-16.982	498.578	671.560	-140.312
298.15	386.887	632.594	632.594	0.000	492.088	705.482	-123.595
300	389.490	634.995	632.601	0.718	491.849	706.804	-123.063
350	457.940	700.228	637.597	21.921	485.881	743.116	-110.902
400	521.430	765.585	649.513	46.429	480.716	780.215	-101.884
450	578.958	830.382	666.018	73.964	476.262	817.925	-94.940
500	630.400	894.096	685.651	104.223	472.423	856.121	-89.437
600	716.730	1016.974	730.724	171.750	466.249	933.474	-81.264
700	785.101	1132.792	779.976	246.971	461.838	1011.724	-75.494
800	840.029	1241.342	830.937	328.324	458.983	1090.480	-71.200
900	884.869	1342.958	882.245	414.641	457.485	1169.503	-67.875
1000	921.972	1438.168	933.128	505.040	457.158	1248.644	-65.221
1100	953.000	1527.539	983.145	598.834	457.781	1327.780	-63.050
1200	979.165	1611.615	1032.049	695.478	459.193	1406.804	-61.235
1300	1001.386	1690.891	1079.710	794.536	461.191	1485.697	-59.695
1400	1020.373	1765.815	1126.066	895.648	463.628	1564.423	-58.368
1500	1036.689	1836.783	1171.102	998.521	466.409	1642.965	-57.212
1600	1050.783	1904.151	1214.831	1102.912	469.391	1721.303	-56.194
1700	1063.018	1968.230	1257.279	1208.616	472.489	1799.425	-55.288
1800	1073.690	2029.299	1298.486	1315.463	475.620	1877.433	-54.481
1900	1083.041	2087.606	1338.496	1423.310	478.749	1955.210	-53.751
2000	1091.271	2143.373	1377.356	1532.034	481.813	2032.852	-53.092
2100	1098.545	2196.796	1415.113	1641.532	484.727	2110.328	-52.490
2200	1104.998	2248.052	1451.817	1751.716	487.490	2187.672	-51.941
2300	1110.746	2297.300	1487.514	1862.509	490.093	2264.893	-51.436
2400	1115.884	2344.684	1522.248	1973.845	492.461	2341.952	-50.970
2500	1120.493	2390.331	1556.064	2085.668	494.604	2419.043	-50.542
2600	1124.640	2434.360	1589.003	2197.928	496.482	2495.923	-50.143
2700	1128.384	2476.876	1621.105	2310.582	498.100	2572.816	-49.773
2800	1131.774	2517.975	1652.406	2423.593	499.430	2649.679	-49.429
2900	1134.853	2557.745	1682.942	2536.927	500.438	2726.441	-49.107
3000	1137.655	2596.266	1712.748	2650.554	501.172	2803.201	-48.807
3100	1140.214	2633.612	1741.854	2764.450	501.548	2879.859	-48.524
3200	1142.555	2669.850	1770.290	2878.590	501.610	2956.590	-48.260
3300	1144.702	2705.041	1798.085	2992.954	501.338	3033.368	-48.013
3400	1146.676	2739.244	1825.266	3107.524	500.702	3110.064	-47.779
3500	1148.494	2772.510	1851.857	3222.284	499.707	3186.763	-47.559
3600	1150.172	2804.888	1877.882	3337.219	498.376	3263.592	-47.353
3700	1151.724	2836.423	1903.365	3452.314	496.676	3340.483	-47.158
3800	1153.162	2867.156	1928.325	3567.560	494.576	3417.357	-46.974
3900	1154.498	2897.128	1952.783	3682.943	492.123	3494.235	-46.799
4000	1155.739	2926.373	1976.759	3798.456	489.298	3571.334	-46.636
4100	1156.895	2954.926	2000.270	3914.088	486.061	3648.426	-46.481
4200	1157.973	2982.817	2023.333	4029.832	482.444	3725.592	-46.334
4300	1158.981	3010.077	2045.965	4145.681	478.430	3802.749	-46.193
4400	1159.923	3036.732	2068.180	4261.626	474.031	3880.107	-46.062
4500	1160.806	3062.809	2089.995	4377.663	469.261	3957.631	-45.938
4600	1161.634	3088.331	2111.421	4493.786	464.064	4035.273	-45.821
4700	1162.412	3113.322	2132.473	4609.988	458.454	4112.907	-45.709
4800	1163.144	3137.802	2153.163	4726.267	452.485	4190.781	-45.604
4900	1163.833	3161.793	2173.504	4842.616	446.075	4268.635	-45.503
5000	1164.482	3185.312	2193.506	4959.032	439.326	4346.831	-45.410

3.508. Phenanthro[2,1-*b*]chrysene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 62243-32-7
Point Group: C_{2v}

Length: 19.03 Å
Width: 9.520 Å
Breadth: 3.884 Å
L/B Ratio: 1.999

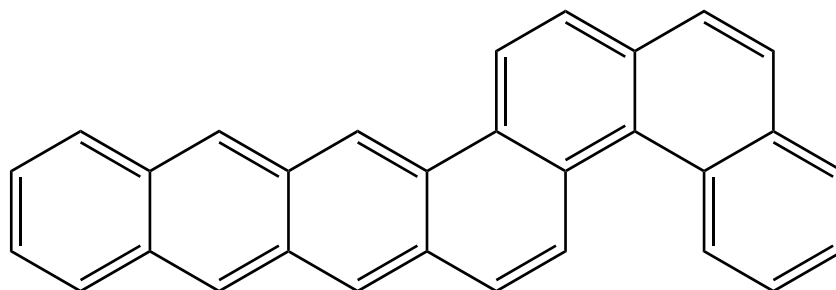
Cartesian coordinates:

C	-7.3632	1.5228	0.0000	C	1.2190	-0.5522	0.0000	H	-6.1539	-1.6749	0.0000
C	-7.3577	0.1132	0.0000	C	1.2171	-1.9700	0.0000	H	-6.1748	3.3130	0.0000
C	-6.1709	-0.5744	0.0000	C	2.4684	-2.6757	0.0000	H	-1.5652	2.1112	0.0000
C	-6.1799	2.2171	0.0000	C	3.6426	-2.0018	0.0000	H	-3.7341	3.3350	0.0000
C	-4.9439	1.5249	0.0000	C	2.4838	0.1518	0.0000	H	-4.5969	-2.5512	0.0000
C	-4.9338	0.1171	0.0000	C	3.6775	-0.5665	0.0000	H	-2.4332	-3.7803	0.0000
C	-2.5240	1.5700	0.0000	C	3.6996	2.2528	0.0000	H	0.0068	-3.7602	0.0000
C	-3.7077	2.2394	0.0000	C	2.5184	1.5791	0.0000	H	-0.0023	1.2351	0.0000
C	-2.4843	0.1429	0.0000	C	4.9384	1.5427	0.0000	H	2.4468	-3.7715	0.0000
C	-3.6755	-0.5797	0.0000	C	4.9334	0.1349	0.0000	H	4.6060	-2.5347	0.0000
C	-3.6354	-2.0150	0.0000	C	6.1729	-0.5521	0.0000	H	3.7221	3.3485	0.0000
C	-2.4588	-2.6846	0.0000	C	7.3573	0.1397	0.0000	H	1.5576	2.1169	0.0000
C	-1.2170	-0.5566	0.0000	C	7.3577	1.5493	0.0000	H	6.1599	-1.6527	0.0000
C	-1.2101	-1.9744	0.0000	C	6.1720	2.2394	0.0000	H	8.3119	-0.3966	0.0000
C	0.0048	-2.6630	0.0000	H	-8.3198	2.0553	0.0000	H	8.3125	2.0852	0.0000
C	-0.0003	0.1283	0.0000	H	-8.3103	-0.4265	0.0000	H	6.1630	3.3353	0.0000

Table 3.508: Table of thermodynamic data as a function of temperature for Phenanthro[2,1-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.132	485.715	485.715	∞
100	126.618	371.332	864.701	-49.337	515.321	571.698	-298.618
200	246.745	493.854	648.730	-30.975	499.656	634.319	-165.664
250	316.757	556.378	623.979	-16.900	492.287	668.838	-139.743
298.15	385.060	618.024	618.024	0.000	485.715	703.453	-123.240
300	387.654	620.414	618.031	0.715	485.473	704.803	-122.715
350	455.902	685.347	623.003	21.820	479.408	741.851	-110.713
400	519.281	750.424	634.866	46.223	474.138	779.702	-101.816
450	576.779	814.965	651.299	73.650	469.575	818.176	-94.969
500	628.248	878.451	670.850	103.800	465.628	857.149	-89.544
600	714.727	1000.948	715.750	171.119	459.245	936.086	-81.492
700	783.290	1116.471	764.830	246.149	454.643	1015.954	-75.810
800	838.406	1224.792	815.629	327.330	451.618	1096.354	-71.583
900	883.418	1326.227	866.789	413.495	449.966	1177.042	-68.312
1000	920.671	1421.292	917.536	503.756	449.501	1257.863	-65.703
1100	951.830	1510.546	967.431	597.426	450.000	1338.693	-63.568
1200	978.111	1594.525	1016.225	693.960	451.302	1419.421	-61.784
1300	1000.433	1673.720	1063.785	792.917	453.200	1500.027	-60.271
1400	1019.509	1748.577	1110.050	893.938	455.546	1580.474	-58.967
1500	1035.903	1819.489	1155.003	996.729	458.244	1660.742	-57.831
1600	1050.066	1886.807	1198.655	1101.044	461.151	1740.813	-56.831
1700	1062.362	1950.845	1241.033	1206.680	464.180	1820.670	-55.941
1800	1073.089	2011.878	1282.176	1313.465	467.249	1900.419	-55.148
1900	1082.489	2070.154	1322.126	1421.254	470.320	1979.939	-54.431
2000	1090.762	2125.894	1360.931	1529.925	473.331	2059.328	-53.783
2100	1098.074	2179.293	1398.638	1639.374	476.196	2138.553	-53.192
2200	1104.562	2230.528	1435.295	1749.512	478.913	2217.649	-52.653
2300	1110.341	2279.757	1470.948	1860.263	481.475	2296.623	-52.157
2400	1115.507	2327.124	1505.641	1971.560	483.803	2375.437	-51.699
2500	1120.141	2372.757	1539.419	2083.346	485.910	2454.284	-51.278
2600	1124.312	2416.773	1572.322	2195.573	487.754	2532.923	-50.886
2700	1128.077	2459.276	1604.389	2308.195	489.341	2611.575	-50.523
2800	1131.486	2500.364	1635.659	2421.176	490.641	2690.199	-50.185
2900	1134.582	2540.125	1666.165	2534.482	491.620	2768.722	-49.869
3000	1137.401	2578.637	1695.942	2648.083	492.329	2847.245	-49.574
3100	1139.974	2615.975	1725.022	2761.954	492.679	2925.666	-49.296
3200	1142.328	2652.205	1753.433	2876.071	492.718	3004.161	-49.037
3300	1144.487	2687.390	1781.204	2990.413	492.425	3082.704	-48.794
3400	1146.473	2721.586	1808.362	3104.963	491.768	3161.165	-48.564
3500	1148.301	2754.846	1834.931	3219.702	490.753	3239.631	-48.348
3600	1149.989	2787.219	1860.936	3334.618	489.403	3318.226	-48.145
3700	1151.551	2818.749	1886.399	3449.696	487.686	3396.884	-47.954
3800	1152.997	2849.478	1911.340	3564.924	485.569	3475.525	-47.773
3900	1154.340	2879.446	1935.781	3680.292	483.100	3554.172	-47.602
4000	1155.589	2908.687	1959.740	3795.789	480.259	3633.039	-47.442
4100	1156.752	2937.236	1983.234	3911.407	477.007	3711.900	-47.289
4200	1157.837	2965.124	2006.282	4027.137	473.377	3790.835	-47.145
4300	1158.850	2992.380	2028.899	4142.972	469.349	3869.762	-47.007
4400	1159.798	3019.033	2051.100	4258.905	464.937	3948.889	-46.878
4500	1160.686	3045.107	2072.900	4374.930	460.155	4028.184	-46.757
4600	1161.519	3070.627	2094.313	4491.040	454.946	4107.596	-46.642
4700	1162.302	3095.615	2115.353	4607.232	449.325	4187.000	-46.532
4800	1163.038	3120.093	2136.031	4723.499	443.346	4266.646	-46.430
4900	1163.731	3144.081	2156.359	4839.838	436.924	4346.270	-46.331
5000	1164.384	3167.599	2176.350	4956.244	430.165	4426.238	-46.240

3.509. Phenanthro[3,4-*a*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-89-2
Point Group: C₁

Length: 19.21 Å
Width: 9.372 Å
Breadth: 5.049 Å
L/B Ratio: 2.050

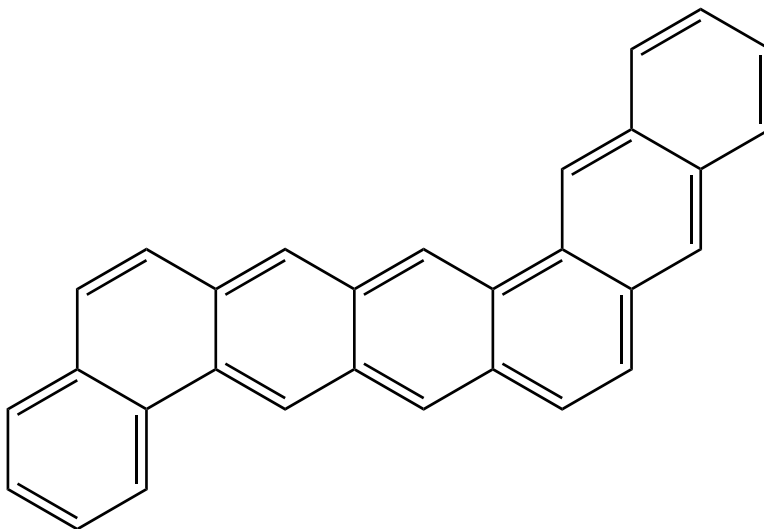
Cartesian coordinates:

C	7.7646	-0.9238	-0.3936	C	-0.8197	-0.7345	0.1163	H	6.9611	2.3524	0.1985
C	7.9269	0.4781	-0.1702	C	-1.9395	0.1036	0.1982	H	6.3929	-2.5560	-0.5837
C	6.8468	1.2762	0.0264	C	-2.2418	-2.6830	0.0820	H	4.5243	2.6054	0.3852
C	6.5275	-1.4818	-0.4131	C	-0.9914	-2.1367	0.0272	H	3.9566	-2.3043	-0.3985
C	5.3568	-0.6736	-0.2095	C	-3.3852	-1.8481	0.1185	H	2.0868	2.8511	0.5782
C	5.5190	0.7267	0.0137	C	-3.2563	-0.4485	0.0599	H	1.5233	-2.0558	-0.2130
C	4.4031	1.5287	0.2133	C	-5.8005	-1.7209	0.2443	H	-0.3311	3.0800	0.8604
C	4.0839	-1.2283	-0.2267	C	-4.6733	-2.4682	0.2377	H	-2.5836	2.1339	0.7112
C	2.9491	-0.4217	-0.0255	C	-5.7244	-0.3085	0.0120	H	-2.3751	-3.7712	0.0839
C	3.1111	0.9730	0.1976	C	-4.4720	0.3232	-0.1404	H	-0.0989	-2.7758	-0.0531
C	1.9601	1.7757	0.4017	C	-4.4786	1.6719	-0.5657	H	-6.7863	-2.1788	0.3846
C	1.6432	-0.9739	-0.0424	C	-5.6517	2.3716	-0.7298	H	-4.7178	-3.5582	0.3462
C	0.5290	-0.1841	0.1494	C	-6.8879	1.7554	-0.4813	H	-3.5282	2.1764	-0.7865
C	0.7000	1.2183	0.3801	C	-6.9220	0.4280	-0.1271	H	-5.6272	3.4152	-1.0609
C	-0.4745	2.0237	0.6036	H	8.6595	-1.5353	-0.5482	H	-7.8136	2.3294	-0.5891
C	-1.7118	1.4957	0.5111	H	8.9405	0.8919	-0.1615	H	-7.8802	-0.0781	0.0381

Table 3.509: Table of thermodynamic data as a function of temperature for Phenanthro[3,4-*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.835	532.742	532.742	∞
100	124.511	372.493	864.956	-49.246	562.437	618.698	-323.168
200	246.386	494.131	649.141	-31.002	546.656	681.263	-177.924
250	317.064	556.649	624.361	-16.928	539.286	715.769	-149.549
298.15	385.880	618.394	618.394	0.000	532.742	750.369	-131.459
300	388.491	620.789	618.402	0.716	532.501	751.718	-130.883
350	457.115	685.882	623.386	21.874	526.487	788.743	-117.711
400	520.730	751.137	635.278	46.344	521.284	826.563	-107.936
450	578.356	815.858	651.755	73.846	516.798	864.997	-100.404
500	629.877	879.513	671.359	104.077	512.931	903.921	-94.430
600	716.329	1002.307	716.376	171.559	506.711	982.737	-85.553
700	784.788	1118.070	765.579	246.744	502.265	1062.456	-79.280
800	839.782	1226.582	816.496	328.069	499.382	1142.686	-74.608
900	884.672	1328.172	867.767	414.365	497.862	1223.187	-70.990
1000	921.813	1423.364	918.618	504.746	497.517	1303.807	-68.103
1100	952.869	1512.722	968.608	598.525	498.125	1384.425	-65.739
1200	979.057	1596.786	1017.489	695.157	499.526	1464.930	-63.765
1300	1001.295	1676.055	1065.128	794.205	501.514	1545.307	-62.090
1400	1020.297	1750.972	1111.466	895.309	503.942	1625.517	-60.648
1500	1036.623	1821.936	1156.486	998.175	506.717	1705.544	-59.391
1600	1050.726	1889.299	1200.200	1102.559	509.692	1785.367	-58.285
1700	1062.968	1953.375	1242.635	1208.258	512.785	1864.973	-57.302
1800	1073.647	2014.442	1283.830	1315.101	515.912	1944.468	-56.426
1900	1083.003	2072.747	1323.829	1422.944	519.036	2023.730	-55.635
2000	1091.237	2128.512	1362.680	1531.664	522.097	2102.858	-54.920
2100	1098.514	2181.933	1400.429	1641.159	525.008	2181.820	-54.269
2200	1104.971	2233.188	1437.124	1751.340	527.767	2260.651	-53.674
2300	1110.721	2282.435	1472.813	1862.130	530.369	2339.358	-53.127
2400	1115.862	2329.817	1507.541	1973.464	532.733	2417.903	-52.623
2500	1120.472	2375.464	1541.351	2085.285	534.874	2496.481	-52.160
2600	1124.621	2419.492	1574.284	2197.543	536.750	2574.848	-51.728
2700	1128.367	2462.007	1606.379	2310.195	538.367	2653.228	-51.329
2800	1131.758	2503.106	1637.676	2423.204	539.695	2731.578	-50.957
2900	1134.838	2542.875	1668.207	2536.537	540.701	2809.826	-50.609
3000	1137.642	2581.396	1698.008	2650.163	541.434	2888.074	-50.285
3100	1140.201	2618.741	1727.110	2764.057	541.809	2966.218	-49.979
3200	1142.543	2654.979	1755.543	2878.196	541.869	3044.437	-49.694
3300	1144.691	2690.170	1783.334	2992.559	541.597	3122.701	-49.427
3400	1146.665	2724.372	1810.511	3107.128	540.960	3200.885	-49.175
3500	1148.484	2757.638	1837.099	3221.887	539.963	3279.071	-48.936
3600	1150.163	2790.015	1863.121	3336.820	538.632	3357.387	-48.713
3700	1151.716	2821.550	1888.600	3451.915	536.931	3435.766	-48.503
3800	1153.154	2852.284	1913.557	3567.160	534.830	3514.126	-48.304
3900	1154.490	2882.255	1938.013	3682.543	532.376	3592.492	-48.115
4000	1155.732	2911.500	1961.986	3798.054	529.550	3671.078	-47.938
4100	1156.888	2940.052	1985.495	3913.686	526.313	3749.658	-47.770
4200	1157.967	2967.944	2008.556	4029.429	522.695	3828.311	-47.611
4300	1158.974	2995.203	2031.185	4145.277	518.681	3906.956	-47.459
4400	1159.917	3021.858	2053.399	4261.222	514.281	3985.801	-47.316
4500	1160.800	3047.935	2075.211	4377.258	509.510	4064.812	-47.182
4600	1161.629	3073.457	2096.635	4493.380	504.312	4143.942	-47.055
4700	1162.407	3098.448	2117.686	4609.583	498.702	4223.063	-46.933
4800	1163.139	3122.928	2138.374	4725.860	492.733	4302.425	-46.819
4900	1163.828	3146.918	2158.713	4842.209	486.322	4381.765	-46.709
5000	1164.477	3170.438	2178.713	4958.624	479.572	4461.449	-46.607

3.510. Benzo[*o*]hexaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-76-7
Point Group: C_s

Length: 20.07 Å
Width: 9.855 Å
Breadth: 3.884 Å
L/B Ratio: 2.037

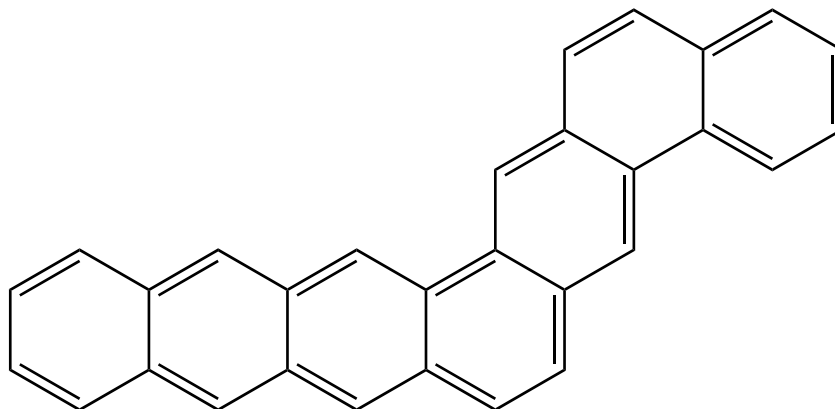
Cartesian coordinates:

C	7.2308	-0.9214	0.0000	C	-1.4687	0.5233	0.0000	H	7.4582	2.4695	0.0000
C	7.8047	0.3345	0.0000	C	-0.9045	1.8386	0.0000	H	4.9725	2.2428	0.0000
C	6.9957	1.4771	0.0000	C	-1.7859	2.9886	0.0000	H	3.4294	-3.5180	0.0000
C	5.6209	1.3531	0.0000	C	-3.1237	2.8466	0.0000	H	5.8940	-3.2443	0.0000
C	5.8314	-1.0621	0.0000	C	-2.9208	0.3724	0.0000	H	3.1711	2.0482	0.0000
C	5.0170	0.0829	0.0000	C	-3.7434	1.5370	0.0000	H	1.1994	-2.5479	0.0000
C	3.8876	-2.5221	0.0000	C	-5.1200	1.4131	0.0000	H	0.8999	3.0110	0.0000
C	5.2280	-2.3736	0.0000	C	-3.5113	-0.8775	0.0000	H	-1.0704	-1.5857	0.0000
C	3.0076	-1.3757	0.0000	C	-4.9156	-1.0170	0.0000	H	-1.3234	3.9826	0.0000
C	3.5697	-0.0634	0.0000	C	-5.7278	0.1390	0.0000	H	-3.7848	3.7212	0.0000
C	2.7322	1.0373	0.0000	C	-7.1454	-0.0074	0.0000	H	-5.7556	2.3075	0.0000
C	1.6342	-1.5407	0.0000	C	-7.7097	-1.2510	0.0000	H	-2.8738	-1.7764	0.0000
C	0.7745	-0.4211	0.0000	C	-6.8943	-2.4112	0.0000	H	-7.7682	0.8943	0.0000
C	1.3297	0.8823	0.0000	C	-5.5330	-2.3013	0.0000	H	-8.7983	-1.3693	0.0000
C	0.4632	2.0046	0.0000	H	7.8612	-1.8179	0.0000	H	-7.3742	-3.3954	0.0000
C	-0.6347	-0.5734	0.0000	H	8.8943	0.4421	0.0000	H	-4.8955	-3.1925	0.0000

Table 3.510: Table of thermodynamic data as a function of temperature for Benzo[*o*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.267	496.901	496.901	∞
100	126.375	382.531	876.435	-49.390	526.453	581.710	-303.848
200	247.066	505.077	660.186	-31.022	510.795	643.214	-167.987
250	317.243	567.691	635.397	-16.926	503.447	677.169	-141.484
298.15	385.658	629.432	629.432	0.000	496.901	711.238	-124.603
300	388.255	631.826	629.440	0.716	496.660	712.566	-124.066
350	456.564	696.858	634.420	21.853	490.627	749.041	-111.786
400	519.961	762.024	646.300	46.290	485.390	786.314	-102.680
450	577.454	826.646	662.756	73.750	480.862	824.206	-95.669
500	628.908	890.202	682.333	103.934	476.947	862.593	-90.113
600	715.360	1012.817	727.287	171.318	470.630	940.350	-81.863
700	783.913	1128.437	776.422	246.410	466.090	1019.026	-76.039
800	839.029	1236.840	827.273	327.654	463.127	1098.224	-71.705
900	884.040	1338.349	878.482	413.880	461.537	1177.704	-68.351
1000	921.289	1433.479	929.276	504.204	461.135	1257.310	-65.674
1100	952.436	1522.791	979.214	597.935	461.695	1336.918	-63.484
1200	978.698	1606.822	1028.048	694.528	463.056	1416.418	-61.654
1300	1000.997	1686.064	1075.646	793.543	465.012	1495.793	-60.100
1400	1020.048	1760.961	1121.947	894.620	467.413	1575.003	-58.763
1500	1036.414	1831.909	1166.934	997.463	470.164	1654.031	-57.597
1600	1050.549	1899.260	1210.617	1101.828	473.120	1732.858	-56.571
1700	1062.817	1963.326	1253.026	1207.511	476.197	1811.469	-55.659
1800	1073.517	2024.385	1294.196	1314.339	479.310	1889.969	-54.844
1900	1082.891	2082.683	1334.173	1422.170	482.422	1968.237	-54.109
2000	1091.140	2138.443	1373.002	1530.880	485.472	2046.371	-53.445
2100	1098.429	2191.859	1410.733	1640.366	488.374	2124.341	-52.839
2200	1104.896	2243.111	1447.411	1750.539	491.126	2202.179	-52.285
2300	1110.655	2292.355	1483.084	1861.322	493.720	2279.894	-51.777
2400	1115.803	2339.734	1517.797	1972.649	496.079	2357.448	-51.307
2500	1120.419	2385.379	1551.593	2084.464	498.214	2435.034	-50.876
2600	1124.574	2429.405	1584.514	2196.718	500.085	2512.410	-50.474
2700	1128.324	2471.918	1616.598	2309.366	501.697	2589.798	-50.102
2800	1131.720	2513.015	1647.883	2422.371	503.021	2667.157	-49.755
2900	1134.803	2552.783	1678.404	2535.699	504.024	2744.415	-49.431
3000	1137.609	2591.303	1708.196	2649.322	504.753	2821.671	-49.129
3100	1140.171	2628.647	1737.288	2763.213	505.124	2898.825	-48.844
3200	1142.516	2664.884	1765.712	2877.349	505.182	2976.053	-48.578
3300	1144.666	2700.074	1793.496	2991.710	504.907	3053.327	-48.329
3400	1146.642	2734.276	1820.665	3106.276	504.268	3130.520	-48.094
3500	1148.462	2767.541	1847.246	3221.033	503.269	3207.716	-47.872
3600	1150.143	2799.918	1873.261	3335.964	501.935	3285.042	-47.664
3700	1151.697	2831.452	1898.734	3451.057	500.232	3362.430	-47.468
3800	1153.137	2862.185	1923.685	3566.300	498.130	3439.801	-47.282
3900	1154.473	2892.156	1948.135	3681.681	495.674	3517.176	-47.106
4000	1155.716	2921.400	1972.103	3797.191	492.847	3594.773	-46.942
4100	1156.874	2949.953	1995.606	3912.822	489.608	3672.362	-46.785
4200	1157.953	2977.843	2018.662	4028.564	485.989	3750.025	-46.637
4300	1158.962	3005.103	2041.286	4144.410	481.973	3827.680	-46.496
4400	1159.905	3031.758	2063.495	4260.354	477.572	3905.535	-46.364
4500	1160.789	3057.834	2085.303	4376.389	472.800	3983.557	-46.239
4600	1161.618	3083.356	2106.723	4492.510	467.601	4061.696	-46.121
4700	1162.397	3108.346	2127.770	4608.711	461.990	4139.828	-46.008
4800	1163.129	3132.827	2148.454	4724.987	456.020	4218.199	-45.902
4900	1163.819	3156.817	2168.789	4841.335	449.607	4296.550	-45.801
5000	1164.469	3180.335	2188.786	4957.750	442.857	4375.245	-45.707

3.511. Benzo[*c*]hexaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-92-7
Point Group: C_s

Length: 20.33 Å
Width: 9.876 Å
Breadth: 3.884 Å
L/B Ratio: 2.058

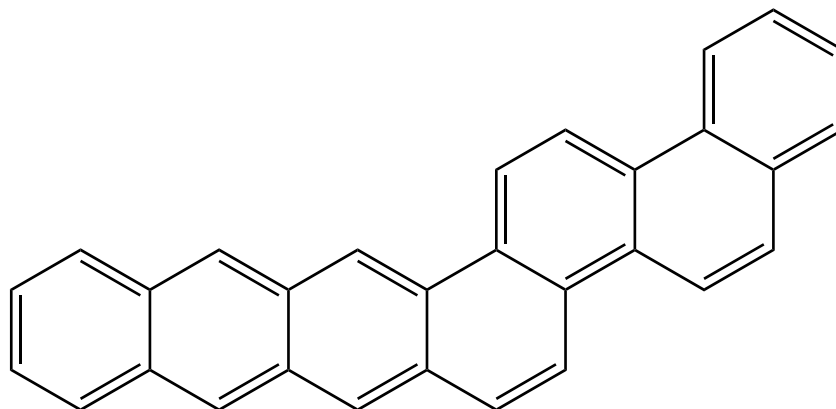
Cartesian coordinates:

C	7.4509	-2.0163	0.0000	C	-0.7949	0.4179	0.0000	H	7.5133	1.4071	0.0000
C	7.9669	-0.6854	0.0000	C	-1.6507	1.5472	0.0000	H	5.7054	-3.2562	0.0000
C	7.1265	0.3817	0.0000	C	-3.0290	1.3712	0.0000	H	5.2232	2.2960	0.0000
C	6.1109	-2.2381	0.0000	C	-1.3505	-0.8564	0.0000	H	3.4144	-2.3691	0.0000
C	5.1886	-1.1380	0.0000	C	-2.7407	-1.0380	0.0000	H	2.9344	3.1807	0.0000
C	5.7037	0.1907	0.0000	C	-3.5920	0.0870	0.0000	H	1.1163	-1.4807	0.0000
C	4.8282	1.2726	0.0000	C	-4.6475	-2.5420	0.0000	H	0.6782	4.0772	0.0000
C	3.8126	-1.3470	0.0000	C	-3.3069	-2.3608	0.0000	H	-1.7734	3.7281	0.0000
C	2.9267	-0.2590	0.0000	C	-5.5445	-1.4174	0.0000	H	-3.7046	2.2421	0.0000
C	3.4404	1.0665	0.0000	C	-5.0270	-0.1104	0.0000	H	-0.6803	-1.7314	0.0000
C	2.5307	2.1605	0.0000	C	-5.9192	0.9815	0.0000	H	-5.0815	-3.5485	0.0000
C	1.5181	-0.4544	0.0000	C	-7.2805	0.7735	0.0000	H	-2.6212	-3.2159	0.0000
C	0.6512	0.6121	0.0000	C	-7.7949	-0.5325	0.0000	H	-5.4997	1.9993	0.0000
C	1.1727	1.9493	0.0000	C	-6.9409	-1.6135	0.0000	H	-7.9685	1.6251	0.0000
C	0.2513	3.0674	0.0000	H	8.1583	-2.8520	0.0000	H	-8.8791	-0.6853	0.0000
C	-1.0810	2.8781	0.0000	H	9.0527	-0.5449	0.0000	H	-7.3381	-2.6349	0.0000

Table 3.511: Table of thermodynamic data as a function of temperature for Benzo[*c*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.588	501.850	501.850	∞
100	127.238	386.823	882.805	-49.598	531.194	586.022	-306.100
200	248.107	510.001	665.688	-31.137	515.629	647.062	-168.992
250	318.429	572.864	640.809	-16.986	508.336	680.765	-142.235
298.15	386.946	634.824	634.824	0.000	501.850	714.579	-125.189
300	389.546	637.225	634.831	0.718	501.612	715.898	-124.646
350	457.907	702.460	639.827	21.922	495.644	752.098	-112.242
400	521.308	767.807	651.743	46.426	490.475	789.086	-103.042
450	578.770	832.586	668.246	73.953	486.013	826.685	-95.957
500	630.170	896.278	687.875	104.201	482.164	864.771	-90.340
600	716.482	1019.110	732.937	171.704	475.965	941.909	-81.999
700	784.888	1134.892	782.176	246.901	471.531	1019.947	-76.108
800	839.871	1243.417	833.123	328.236	468.658	1098.494	-71.723
900	884.768	1345.018	884.417	414.540	467.147	1177.311	-68.328
1000	921.920	1440.220	935.289	504.932	466.812	1256.246	-65.618
1100	952.986	1529.589	985.296	598.722	467.432	1335.177	-63.401
1200	979.181	1613.664	1034.192	695.367	468.844	1413.996	-61.548
1300	1001.424	1692.942	1081.845	794.427	470.845	1492.684	-59.976
1400	1020.426	1767.869	1128.195	895.544	473.286	1571.205	-58.621
1500	1036.752	1838.842	1173.227	998.423	476.073	1649.541	-57.441
1600	1050.852	1906.214	1216.951	1102.820	479.061	1727.673	-56.402
1700	1063.090	1970.297	1259.396	1208.531	482.167	1805.588	-55.478
1800	1073.764	2031.371	1300.601	1315.386	485.305	1883.390	-54.653
1900	1083.116	2089.682	1340.608	1423.240	488.442	1960.959	-53.909
2000	1091.345	2145.452	1379.466	1531.972	491.513	2038.393	-53.236
2100	1098.617	2198.879	1417.223	1641.477	494.435	2115.661	-52.623
2200	1105.069	2250.138	1453.926	1751.668	497.204	2192.797	-52.063
2300	1110.814	2299.390	1489.621	1862.468	499.815	2269.808	-51.548
2400	1115.950	2346.776	1524.355	1973.810	502.189	2346.658	-51.073
2500	1120.556	2392.426	1558.170	2085.640	504.338	2423.540	-50.636
2600	1124.701	2436.458	1591.109	2197.906	506.223	2500.211	-50.229
2700	1128.442	2478.975	1623.210	2310.567	507.847	2576.894	-49.852
2800	1131.830	2520.077	1654.511	2423.583	509.182	2653.547	-49.502
2900	1134.906	2559.848	1685.048	2536.922	510.196	2730.098	-49.173
3000	1137.706	2598.371	1714.853	2650.555	510.935	2806.648	-48.867
3100	1140.262	2635.719	1743.959	2764.455	511.316	2883.095	-48.579
3200	1142.601	2671.958	1772.396	2878.600	511.383	2959.616	-48.310
3300	1144.746	2707.151	1800.191	2992.969	511.116	3036.182	-48.058
3400	1146.718	2741.355	1827.372	3107.544	510.484	3112.667	-47.819
3500	1148.535	2774.622	1853.963	3222.308	509.493	3189.156	-47.595
3600	1150.211	2807.001	1879.988	3337.246	508.167	3265.773	-47.384
3700	1151.762	2838.537	1905.471	3452.346	506.470	3342.453	-47.186
3800	1153.199	2869.272	1930.431	3567.595	504.374	3419.115	-46.998
3900	1154.532	2899.244	1954.890	3682.982	501.924	3495.781	-46.820
4000	1155.772	2928.490	1978.866	3798.498	499.102	3572.669	-46.653
4100	1156.927	2957.044	2002.377	3914.134	495.869	3649.549	-46.495
4200	1158.004	2984.936	2025.441	4029.881	492.255	3726.503	-46.345
4300	1159.010	3012.196	2048.073	4145.732	488.244	3803.449	-46.202
4400	1159.951	3038.852	2070.289	4261.681	483.848	3880.594	-46.068
4500	1160.833	3064.930	2092.103	4377.720	479.081	3957.906	-45.941
4600	1161.661	3090.453	2113.530	4493.845	473.886	4035.336	-45.822
4700	1162.437	3115.444	2134.582	4610.051	468.279	4112.758	-45.707
4800	1163.168	3139.925	2155.273	4726.331	462.313	4190.420	-45.600
4900	1163.856	3163.916	2175.613	4842.683	455.904	4268.061	-45.497
5000	1164.505	3187.435	2195.615	4959.101	449.158	4346.045	-45.402

3.512. Naphtho[2,3-*b*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-75-6
Point Group: C_s

Length: 20.31 Å
Width: 9.484 Å
Breadth: 3.884 Å
L/B Ratio: 2.142

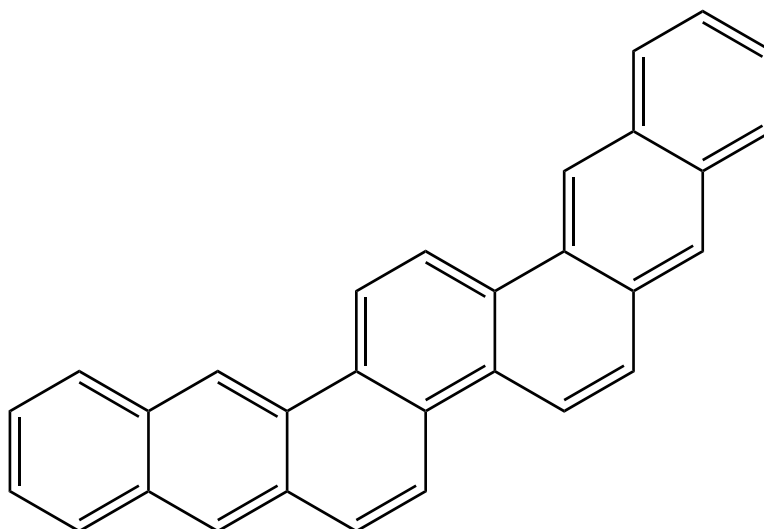
Cartesian coordinates:

C	7.6276	-1.8337	0.0000	C	-0.7579	0.0670	0.0000	H	7.4699	1.5874	0.0000
C	8.0569	-0.4710	0.0000	C	-1.6813	1.1147	0.0000	H	5.9669	-3.1840	0.0000
C	7.1503	0.5392	0.0000	C	-2.5613	-1.5488	0.0000	H	5.1270	2.3262	0.0000
C	6.3057	-2.1418	0.0000	C	-1.2222	-1.2714	0.0000	H	3.6237	-2.4467	0.0000
C	5.3124	-1.1035	0.0000	C	-3.5178	-0.5036	0.0000	H	2.7842	3.0600	0.0000
C	5.7411	0.2576	0.0000	C	-3.0808	0.8294	0.0000	H	1.2777	-1.7105	0.0000
C	4.8001	1.2791	0.0000	C	-4.0549	1.8836	0.0000	H	0.4647	3.8024	0.0000
C	3.9558	-1.4012	0.0000	C	-5.3833	1.6160	0.0000	H	-1.9582	3.2794	0.0000
C	2.9976	-0.3716	0.0000	C	-4.9328	-0.7958	0.0000	H	-2.9242	-2.5882	0.0000
C	3.4249	0.9845	0.0000	C	-5.8574	0.2632	0.0000	H	-0.4781	-2.0828	0.0000
C	2.4502	2.0149	0.0000	C	-7.2424	-0.0163	0.0000	H	-3.6885	2.9214	0.0000
C	1.6092	-0.6595	0.0000	C	-7.6875	-1.3174	0.0000	H	-6.1213	2.4264	0.0000
C	0.6700	0.3496	0.0000	C	-6.7659	-2.3794	0.0000	H	-7.9547	0.8165	0.0000
C	1.1052	1.7149	0.0000	C	-5.4150	-2.1243	0.0000	H	-8.7603	-1.5358	0.0000
C	0.1131	2.7641	0.0000	H	8.3881	-2.6213	0.0000	H	-7.1331	-3.4108	0.0000
C	-1.2044	2.4774	0.0000	H	9.1315	-0.2614	0.0000	H	-4.6835	-2.9467	0.0000

Table 3.512: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*b*]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-57.761	507.901	507.901	∞
100	127.987	385.073	882.599	-49.753	537.091	592.094	-309.272
200	248.828	508.724	664.843	-31.224	521.593	653.282	-170.616
250	319.315	571.765	639.896	-17.033	514.341	687.044	-143.547
298.15	387.986	633.894	633.894	0.000	507.901	720.907	-126.297
300	390.592	636.302	633.901	0.720	507.664	722.227	-125.748
350	459.065	701.707	638.910	21.979	501.752	758.469	-113.193
400	522.524	767.213	650.857	46.542	496.643	795.491	-103.878
450	579.993	832.136	667.400	74.131	492.242	833.116	-96.704
500	631.362	895.955	687.076	104.440	488.453	871.222	-91.014
600	717.543	1018.995	732.236	172.056	482.368	948.381	-82.562
700	785.781	1134.928	781.570	247.351	478.031	1026.422	-76.591
800	840.599	1243.561	832.604	328.766	475.239	1104.960	-72.145
900	885.350	1345.239	883.977	415.136	473.794	1183.758	-68.702
1000	922.381	1440.496	934.917	505.579	473.511	1262.668	-65.954
1100	953.350	1529.904	984.985	599.411	474.171	1341.570	-63.705
1200	979.469	1614.007	1033.934	696.088	475.616	1420.355	-61.825
1300	1001.651	1693.306	1081.634	795.174	477.643	1499.008	-60.230
1400	1020.606	1768.248	1128.026	896.311	480.104	1577.492	-58.856
1500	1036.895	1839.232	1173.095	999.206	482.907	1655.790	-57.659
1600	1050.966	1906.612	1216.852	1103.616	485.908	1733.883	-56.604
1700	1063.182	1970.702	1259.327	1209.337	489.024	1811.757	-55.667
1800	1073.837	2031.780	1300.557	1316.200	492.171	1889.518	-54.831
1900	1083.175	2090.095	1340.589	1424.061	495.313	1967.046	-54.077
2000	1091.393	2145.868	1379.469	1532.798	498.390	2044.439	-53.394
2100	1098.655	2199.296	1417.245	1642.308	501.316	2121.665	-52.772
2200	1105.100	2250.557	1453.966	1752.502	504.089	2198.759	-52.204
2300	1110.839	2299.810	1489.678	1863.304	506.702	2275.729	-51.682
2400	1115.970	2347.197	1524.427	1974.649	509.079	2352.537	-51.201
2500	1120.572	2392.849	1558.256	2086.481	511.230	2429.376	-50.758
2600	1124.714	2436.880	1591.208	2198.748	513.116	2506.005	-50.345
2700	1128.453	2479.399	1623.321	2311.410	514.741	2582.645	-49.963
2800	1131.838	2520.500	1654.633	2424.427	516.078	2659.256	-49.608
2900	1134.912	2560.272	1685.180	2537.767	517.092	2735.765	-49.275
3000	1137.711	2598.795	1714.995	2651.401	517.832	2812.273	-48.965
3100	1140.266	2636.143	1744.110	2765.301	518.213	2888.677	-48.673
3200	1142.604	2672.382	1772.555	2879.447	518.280	2965.155	-48.400
3300	1144.748	2707.576	1800.359	2993.816	518.013	3041.680	-48.145
3400	1146.719	2741.779	1827.547	3108.390	517.382	3118.122	-47.903
3500	1148.535	2775.046	1854.145	3223.154	516.391	3194.568	-47.675
3600	1150.211	2807.425	1880.178	3338.093	515.064	3271.143	-47.462
3700	1151.761	2838.962	1905.666	3453.192	513.368	3347.780	-47.261
3800	1153.198	2869.696	1930.633	3568.441	511.272	3424.400	-47.071
3900	1154.531	2899.669	1955.097	3683.829	508.822	3501.024	-46.890
4000	1155.771	2928.915	1979.079	3799.344	506.000	3577.869	-46.721
4100	1156.925	2957.468	2002.595	3914.980	502.766	3654.707	-46.561
4200	1158.002	2985.360	2025.663	4030.727	499.152	3731.619	-46.409
4300	1159.008	3012.620	2048.300	4146.578	495.141	3808.522	-46.263
4400	1159.950	3039.276	2070.520	4262.526	490.745	3885.625	-46.127
4500	1160.831	3065.354	2092.339	4378.566	485.977	3962.894	-45.999
4600	1161.658	3090.877	2113.770	4494.691	480.782	4040.282	-45.878
4700	1162.435	3115.868	2134.826	4610.896	475.175	4117.661	-45.762
4800	1163.166	3140.349	2155.521	4727.176	469.209	4195.281	-45.653
4900	1163.854	3164.340	2175.865	4843.528	462.800	4272.880	-45.549
5000	1164.502	3187.859	2195.870	4959.946	456.053	4350.822	-45.452

3.513. Dibenzo[*b,n*]picene



Other names: Benzo[*b*]naphtho[2,3-*j*]chrysene

Formula: C₃₀H₁₈

Mass: 378.464 g/mol

CAS Number: 213-44-5

Point Group: C_{2v}

Length: 20.18 Å

Width: 9.163 Å

Breadth: 3.884 Å

L/B Ratio: 2.202

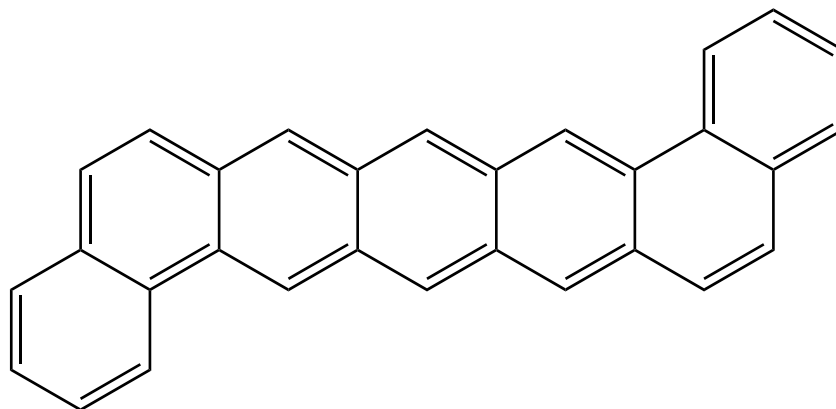
Cartesian coordinates:

C	7.1046	-2.3006	0.0000	C	-1.4088	0.0590	0.0000	H	7.6324	1.0792	0.0000
C	7.7963	-1.0589	0.0000	C	-0.7142	1.2745	0.0000	H	5.2005	-3.2867	0.0000
C	7.1074	0.1173	0.0000	C	-1.4580	2.5093	0.0000	H	5.4816	2.2743	0.0000
C	5.7419	-2.3339	0.0000	C	-2.8081	2.5198	0.0000	H	3.0455	-2.0908	0.0000
C	4.9895	-1.1194	0.0000	C	-2.8615	0.0507	0.0000	H	3.3590	3.4698	0.0000
C	5.6787	0.1177	0.0000	C	-3.5602	1.2905	0.0000	H	0.8797	3.4507	0.0000
C	4.9465	1.3166	0.0000	C	-4.9487	1.3083	0.0000	H	-1.2468	-2.1017	0.0000
C	3.5851	-1.1300	0.0000	C	-3.5832	-1.1360	0.0000	H	1.2503	-2.0996	0.0000
C	2.8614	0.0554	0.0000	C	-4.9876	-1.1277	0.0000	H	-0.8854	3.4492	0.0000
C	3.5580	1.2964	0.0000	C	-5.6789	0.1082	0.0000	H	-3.3647	3.4642	0.0000
C	2.8039	2.5245	0.0000	C	-7.1076	0.1054	0.0000	H	-5.4854	2.2652	0.0000
C	1.4538	2.5117	0.0000	C	-7.7946	-1.0720	0.0000	H	-3.0420	-2.0958	0.0000
C	1.4087	0.0613	0.0000	C	-7.1008	-2.3125	0.0000	H	-7.6342	1.0664	0.0000
C	0.7121	1.2757	0.0000	C	-5.7380	-2.3435	0.0000	H	-8.8895	-1.0800	0.0000
C	-0.6837	-1.1557	0.0000	H	7.6862	-3.2283	0.0000	H	-7.6808	-3.2412	0.0000
C	0.6856	-1.1546	0.0000	H	8.8912	-1.0652	0.0000	H	-5.1950	-3.2953	0.0000

Table 3.513: Table of thermodynamic data as a function of temperature for Dibenzo[*b,n*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.254	499.010	499.010	∞
100	126.562	370.755	865.519	-49.476	528.475	584.910	-305.519
200	247.444	493.491	648.889	-31.080	512.846	647.582	-169.127
250	317.831	556.211	624.053	-16.960	505.521	682.114	-142.517
298.15	386.479	618.076	618.076	0.000	499.010	716.732	-125.566
300	389.085	620.475	618.083	0.717	498.770	718.081	-125.026
350	457.599	685.650	623.074	21.902	492.783	755.121	-112.693
400	521.136	750.965	634.981	46.394	487.602	792.950	-103.547
450	578.702	815.730	651.474	73.915	483.135	831.392	-96.503
500	630.174	879.418	671.094	104.162	479.284	870.321	-90.920
600	716.553	1002.259	716.144	171.669	473.090	949.144	-82.629
700	784.962	1118.053	765.375	246.874	468.663	1028.867	-76.773
800	839.922	1226.587	816.318	328.215	465.797	1109.097	-72.415
900	884.787	1328.191	867.610	414.523	464.289	1189.597	-69.041
1000	921.909	1423.394	918.479	504.915	463.955	1270.214	-66.348
1100	952.952	1512.760	968.485	598.703	464.572	1350.828	-64.144
1200	979.128	1596.832	1017.379	695.343	465.980	1431.330	-62.303
1300	1001.358	1676.105	1065.031	794.397	467.975	1511.702	-60.740
1400	1020.352	1751.027	1111.379	895.507	470.409	1591.907	-59.394
1500	1036.673	1821.995	1156.409	998.379	473.189	1671.927	-58.220
1600	1050.770	1889.361	1200.131	1102.768	476.169	1751.744	-57.187
1700	1063.009	1953.439	1242.574	1208.471	479.266	1831.345	-56.269
1800	1073.683	2014.508	1283.776	1315.318	482.396	1910.832	-55.450
1900	1083.037	2072.815	1323.782	1423.164	485.524	1990.088	-54.710
2000	1091.268	2128.582	1362.638	1531.887	488.588	2069.209	-54.041
2100	1098.542	2182.004	1400.392	1641.385	491.502	2148.164	-53.432
2200	1104.997	2233.261	1437.093	1751.569	494.264	2226.987	-52.874
2300	1110.745	2282.509	1472.787	1862.361	496.868	2305.687	-52.363
2400	1115.884	2329.892	1507.518	1973.697	499.235	2384.225	-51.890
2500	1120.493	2375.540	1541.332	2085.520	501.378	2462.795	-51.456
2600	1124.641	2419.569	1574.269	2197.781	503.256	2541.155	-51.051
2700	1128.385	2462.085	1606.368	2310.435	504.875	2619.527	-50.677
2800	1131.775	2503.184	1637.667	2423.446	506.205	2697.869	-50.328
2900	1134.854	2542.954	1668.202	2536.780	507.212	2776.110	-50.002
3000	1137.656	2581.475	1698.006	2650.407	507.947	2854.350	-49.698
3100	1140.215	2618.821	1727.110	2764.303	508.323	2932.486	-49.411
3200	1142.556	2655.059	1755.545	2878.443	508.385	3010.697	-49.144
3300	1144.703	2690.250	1783.339	2992.808	508.113	3088.953	-48.893
3400	1146.677	2724.453	1810.518	3107.378	507.478	3167.128	-48.656
3500	1148.495	2757.719	1837.108	3222.138	506.483	3245.307	-48.433
3600	1150.173	2790.097	1863.132	3337.072	505.152	3323.615	-48.223
3700	1151.726	2821.632	1888.613	3452.168	503.452	3401.985	-48.026
3800	1153.164	2852.365	1913.572	3567.414	501.352	3480.338	-47.840
3900	1154.499	2882.337	1938.030	3682.798	498.899	3558.695	-47.662
4000	1155.740	2911.582	1962.005	3798.310	496.074	3637.273	-47.497
4100	1156.896	2940.135	1985.515	3913.943	492.838	3715.844	-47.339
4200	1157.975	2968.026	2008.577	4029.687	489.221	3794.489	-47.190
4300	1158.982	2995.286	2031.208	4145.535	485.207	3873.126	-47.048
4400	1159.924	3021.941	2053.423	4261.481	480.808	3951.962	-46.915
4500	1160.807	3048.018	2075.236	4377.518	476.038	4030.966	-46.789
4600	1161.635	3073.540	2096.662	4493.641	470.841	4110.087	-46.671
4700	1162.413	3098.531	2117.713	4609.844	465.231	4189.200	-46.557
4800	1163.145	3123.012	2138.403	4726.122	459.263	4268.553	-46.450
4900	1163.834	3147.002	2158.743	4842.471	452.852	4347.886	-46.348
5000	1164.483	3170.521	2178.744	4958.887	446.103	4427.561	-46.253

3.514. Dibenzo[*a,l*]pentacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 227-09-8
Point Group: C_{2h}

Length: 20.03 Å
Width: 9.136 Å
Breadth: 3.884 Å
L/B Ratio: 2.193

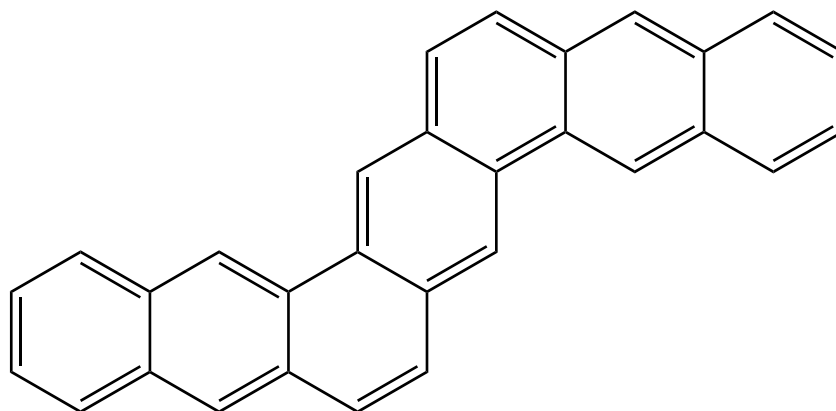
Cartesian coordinates:

C	7.4813	-0.2016	0.0000	C	-1.3358	-0.4439	0.0000	H	7.0597	3.1710	0.0000
C	7.8064	1.1422	0.0000	C	-1.0393	0.9500	0.0000	H	4.6632	2.4746	0.0000
C	6.7960	2.1085	0.0000	C	-2.1143	1.8849	0.0000	H	4.2519	-3.4797	0.0000
C	5.4685	1.7239	0.0000	C	-2.6976	-0.8601	0.0000	H	6.6157	-2.7359	0.0000
C	6.1360	-0.6052	0.0000	C	-3.7220	0.0545	0.0000	H	2.9314	1.9372	0.0000
C	5.1183	0.3636	0.0000	C	-3.4202	1.4598	0.0000	H	1.8785	-2.9564	0.0000
C	4.5092	-2.4140	0.0000	C	-4.5093	2.4140	0.0000	H	0.5215	2.4474	0.0000
C	5.7940	-2.0103	0.0000	C	-5.7941	2.0102	0.0000	H	-0.5213	-2.4473	0.0000
C	3.4202	-1.4597	0.0000	C	-5.1183	-0.3636	0.0000	H	-1.8784	2.9564	0.0000
C	3.7220	-0.0544	0.0000	C	-6.1361	0.6051	0.0000	H	-2.9314	-1.9372	0.0000
C	2.6975	0.8601	0.0000	C	-7.4813	0.2015	0.0000	H	-4.2520	3.4797	0.0000
C	2.1142	-1.8848	0.0000	C	-7.8064	-1.1423	0.0000	H	-6.6158	2.7358	0.0000
C	1.0393	-0.9499	0.0000	C	-6.7959	-2.1085	0.0000	H	-8.2716	0.9608	0.0000
C	1.3358	0.4439	0.0000	C	-5.4683	-1.7239	0.0000	H	-8.8559	-1.4542	0.0000
C	0.2926	1.3745	0.0000	H	8.2715	-0.9610	0.0000	H	-7.0594	-3.1712	0.0000
C	-0.2927	-1.3744	0.0000	H	8.8560	1.4540	0.0000	H	-4.6630	-2.4745	0.0000

Table 3.514: Table of thermodynamic data as a function of temperature for Dibenzo[*a,l*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.870	513.067	513.067	∞
100	125.101	369.998	861.720	-49.172	542.837	599.347	-313.060
200	245.956	491.692	646.320	-30.926	527.057	662.153	-172.933
250	316.268	554.073	621.602	-16.882	519.657	696.783	-145.582
298.15	384.795	615.653	615.653	0.000	513.067	731.512	-128.155
300	387.397	618.041	615.660	0.714	512.824	732.865	-127.601
350	455.804	682.948	620.630	21.811	506.750	770.033	-114.919
400	519.287	748.018	632.489	46.212	501.478	808.004	-105.512
450	576.855	812.565	648.919	73.641	496.918	846.599	-98.269
500	628.376	876.061	668.469	103.796	492.975	885.691	-92.526
600	714.935	998.589	713.369	171.132	486.610	964.866	-83.997
700	783.566	1114.150	762.455	246.186	482.032	1044.968	-77.975
800	838.741	1222.511	813.264	327.398	479.037	1125.598	-73.492
900	883.798	1323.989	864.435	413.598	477.421	1206.512	-70.023
1000	921.081	1419.096	915.196	503.899	476.996	1287.555	-67.254
1100	952.256	1508.389	965.106	597.612	477.537	1368.602	-64.988
1200	978.541	1592.405	1013.915	694.188	478.882	1449.544	-63.096
1300	1000.858	1671.635	1061.491	793.188	480.823	1530.360	-61.489
1400	1019.924	1746.523	1107.772	894.251	483.210	1611.014	-60.106
1500	1036.304	1817.463	1152.741	997.083	485.950	1691.487	-58.902
1600	1050.449	1884.807	1196.408	1101.438	488.896	1771.758	-57.841
1700	1062.727	1948.867	1238.802	1207.111	491.963	1851.815	-56.898
1800	1073.435	2009.921	1279.959	1313.931	495.067	1931.761	-56.057
1900	1082.817	2068.215	1319.924	1421.754	498.171	2011.475	-55.298
2000	1091.072	2123.971	1358.742	1530.457	501.215	2091.057	-54.612
2100	1098.367	2177.385	1396.463	1639.936	504.110	2170.473	-53.986
2200	1104.838	2228.633	1433.132	1750.103	506.855	2249.760	-53.415
2300	1110.602	2277.874	1468.796	1860.880	509.444	2328.922	-52.890
2400	1115.753	2325.252	1503.501	1972.203	511.797	2407.924	-52.406
2500	1120.374	2370.895	1537.289	2084.013	513.928	2486.959	-51.961
2600	1124.531	2414.919	1570.203	2196.262	515.795	2565.783	-51.546
2700	1128.284	2457.431	1602.280	2308.906	517.403	2644.620	-51.162
2800	1131.682	2498.526	1633.559	2421.907	518.723	2723.428	-50.805
2900	1134.768	2538.293	1664.075	2535.232	519.722	2802.135	-50.471
3000	1137.577	2576.812	1693.861	2648.851	520.448	2880.840	-50.159
3100	1140.140	2614.155	1722.949	2762.739	520.816	2959.443	-49.865
3200	1142.486	2650.390	1751.368	2876.872	520.871	3038.121	-49.591
3300	1144.638	2685.580	1779.147	2991.230	520.593	3116.844	-49.335
3400	1146.616	2719.781	1806.312	3105.794	519.951	3195.486	-49.092
3500	1148.438	2753.045	1832.888	3220.548	518.950	3274.132	-48.863
3600	1150.120	2785.421	1858.900	3335.477	517.614	3352.908	-48.648
3700	1151.675	2816.955	1884.369	3450.568	515.908	3431.746	-48.447
3800	1153.116	2847.687	1909.317	3565.808	513.804	3510.566	-48.255
3900	1154.453	2877.658	1933.764	3681.187	511.346	3589.391	-48.074
4000	1155.697	2906.902	1957.728	3796.696	508.516	3668.437	-47.904
4100	1156.855	2935.453	1981.228	3912.324	505.276	3747.476	-47.742
4200	1157.936	2963.344	2004.281	4028.064	501.655	3826.590	-47.590
4300	1158.945	2990.603	2026.903	4143.909	497.637	3905.694	-47.444
4400	1159.889	3017.257	2049.109	4259.851	493.235	3984.999	-47.307
4500	1160.774	3043.333	2070.914	4375.885	488.461	4064.471	-47.178
4600	1161.603	3068.855	2092.332	4492.004	483.261	4144.061	-47.056
4700	1162.383	3093.845	2113.376	4608.204	477.648	4223.642	-46.940
4800	1163.116	3118.325	2134.058	4724.479	471.677	4303.464	-46.830
4900	1163.806	3142.315	2154.391	4840.825	465.263	4383.265	-46.725
5000	1164.456	3165.833	2174.386	4957.239	458.511	4463.410	-46.628

3.515. Naphtho[2,3-*c*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 222-58-2
Point Group: C_{2h}

Length: 20.17 Å
Width: 9.177 Å
Breadth: 3.887 Å
L/B Ratio: 2.198

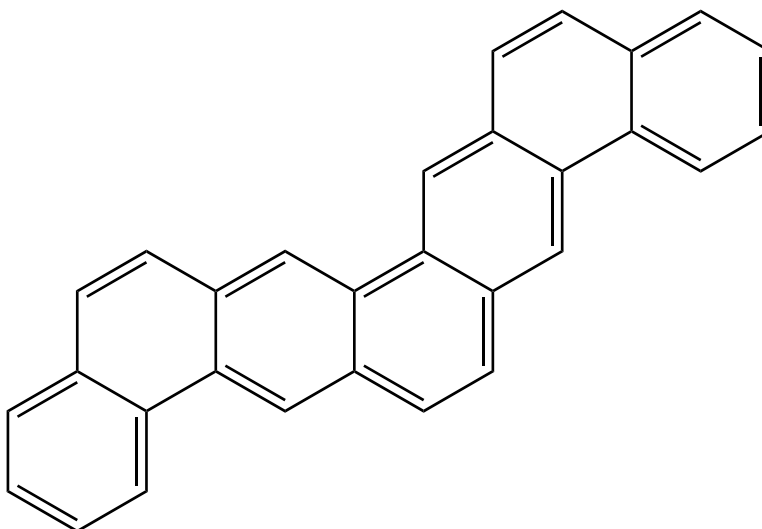
Cartesian coordinates:

C	7.3085	-1.6584	0.0000	C	-0.5908	-1.2716	0.0000	H	7.4920	1.7565	0.0000
C	7.8711	-0.3549	0.0000	C	-1.4033	-0.1159	0.0000	H	5.5120	-2.8308	0.0000
C	7.0663	0.7468	0.0000	C	-2.5459	-2.7183	0.0000	H	5.2341	2.7299	0.0000
C	5.9548	-1.8284	0.0000	C	-1.2051	-2.5792	0.0000	H	3.2435	-1.8558	0.0000
C	5.0864	-0.6963	0.0000	C	-3.4189	-1.5659	0.0000	H	3.0110	3.7111	0.0000
C	5.6466	0.6024	0.0000	C	-2.8520	-0.2588	0.0000	H	0.5454	3.4546	0.0000
C	4.7953	1.7243	0.0000	C	-3.6867	0.8468	0.0000	H	-1.4399	2.0390	0.0000
C	3.6866	-0.8468	0.0000	C	-4.7952	-1.7243	0.0000	H	1.4400	-2.0389	0.0000
C	2.8520	0.2589	0.0000	C	-5.6466	-0.6025	0.0000	H	-3.0109	-3.7110	0.0000
C	3.4189	1.5659	0.0000	C	-5.0864	0.6963	0.0000	H	-0.5454	-3.4545	0.0000
C	2.5460	2.7183	0.0000	C	-5.9549	1.8284	0.0000	H	-3.2435	1.8558	0.0000
C	1.2052	2.5792	0.0000	C	-7.3086	1.6584	0.0000	H	-5.2341	-2.7299	0.0000
C	1.4033	0.1160	0.0000	C	-7.8711	0.3549	0.0000	H	-5.5121	2.8308	0.0000
C	0.5908	1.2717	0.0000	C	-7.0663	-0.7468	0.0000	H	-7.9799	2.5234	0.0000
C	-0.7988	1.1425	0.0000	H	7.9798	-2.5235	0.0000	H	-8.9610	0.2499	0.0000
C	0.7988	-1.1424	0.0000	H	8.9610	-0.2500	0.0000	H	-7.4920	-1.7566	0.0000

Table 3.515: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*c*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.333	491.537	491.537	∞
100	126.444	379.373	873.374	-49.400	521.079	576.652	-301.206
200	247.119	501.977	657.093	-31.023	505.430	638.469	-166.747
250	317.253	564.599	632.304	-16.926	498.083	672.579	-140.525
298.15	385.641	626.339	626.339	0.000	491.537	706.796	-123.825
300	388.238	628.733	626.347	0.716	491.296	708.130	-123.294
350	456.530	693.760	631.326	21.852	485.261	744.760	-111.147
400	519.917	758.921	643.206	46.286	480.023	782.188	-102.141
450	577.405	823.538	659.660	73.745	475.492	820.236	-95.209
500	628.859	887.088	679.236	103.926	471.576	858.778	-89.714
600	715.315	1009.695	724.187	171.305	465.253	936.846	-81.558
700	783.876	1125.308	773.318	246.393	460.710	1015.835	-75.801
800	839.000	1233.708	824.166	327.633	457.743	1095.346	-71.517
900	884.020	1335.213	875.371	413.857	456.151	1175.139	-68.202
1000	921.274	1430.342	926.163	504.179	455.747	1255.059	-65.556
1100	952.426	1519.653	976.099	597.909	456.306	1334.981	-63.392
1200	978.693	1603.683	1024.931	694.502	457.666	1414.795	-61.583
1300	1000.995	1682.924	1072.527	793.516	459.622	1494.483	-60.048
1400	1020.047	1757.822	1118.827	894.593	462.022	1574.008	-58.726
1500	1036.415	1828.770	1163.812	997.436	464.774	1653.350	-57.574
1600	1050.551	1896.121	1207.495	1101.801	467.730	1732.491	-56.559
1700	1062.821	1960.187	1249.902	1207.484	470.807	1811.415	-55.657
1800	1073.521	2021.246	1291.071	1314.313	473.920	1890.229	-54.852
1900	1082.895	2079.544	1331.047	1422.144	477.033	1968.811	-54.125
2000	1091.144	2135.304	1369.876	1530.855	480.083	2047.260	-53.468
2100	1098.433	2188.721	1407.606	1640.341	482.986	2125.543	-52.869
2200	1104.900	2239.972	1444.284	1750.514	485.738	2203.695	-52.321
2300	1110.659	2289.217	1479.957	1861.298	488.332	2281.724	-51.819
2400	1115.807	2336.597	1514.669	1972.626	490.691	2359.591	-51.354
2500	1120.423	2382.241	1548.465	2084.441	492.827	2437.491	-50.928
2600	1124.578	2426.268	1581.385	2196.695	494.699	2515.181	-50.530
2700	1128.328	2468.781	1613.469	2309.343	496.311	2592.883	-50.161
2800	1131.723	2509.878	1644.753	2422.349	497.635	2670.556	-49.819
2900	1134.806	2549.646	1675.275	2535.678	498.638	2748.127	-49.498
3000	1137.613	2588.166	1705.066	2649.301	499.368	2825.697	-49.199
3100	1140.175	2625.511	1734.158	2763.192	499.740	2903.165	-48.917
3200	1142.519	2661.747	1762.582	2877.329	499.798	2980.706	-48.654
3300	1144.669	2696.938	1790.365	2991.689	499.523	3058.294	-48.408
3400	1146.645	2731.139	1817.534	3106.257	498.884	3135.801	-48.175
3500	1148.465	2764.404	1844.115	3221.013	497.886	3213.311	-47.955
3600	1150.146	2796.781	1870.130	3335.945	496.552	3290.950	-47.749
3700	1151.700	2828.316	1895.603	3451.038	494.850	3368.652	-47.556
3800	1153.139	2859.049	1920.554	3566.281	492.748	3446.336	-47.372
3900	1154.476	2889.020	1945.004	3681.663	490.292	3524.025	-47.198
4000	1155.719	2918.264	1968.971	3797.173	487.465	3601.935	-47.035
4100	1156.876	2946.816	1992.474	3912.803	484.226	3679.838	-46.881
4200	1157.955	2974.707	2015.530	4028.546	480.607	3757.815	-46.734
4300	1158.964	3001.967	2038.155	4144.392	476.592	3835.783	-46.595
4400	1159.907	3028.622	2060.363	4260.336	472.191	3913.952	-46.464
4500	1160.791	3054.698	2082.171	4376.372	467.419	3992.287	-46.340
4600	1161.620	3080.220	2103.591	4492.493	462.220	4070.740	-46.224
4700	1162.399	3105.211	2124.637	4608.694	456.609	4149.185	-46.112
4800	1163.131	3129.691	2145.322	4724.971	450.639	4227.871	-46.008
4900	1163.820	3153.681	2165.657	4841.319	444.227	4306.535	-45.907
5000	1164.470	3177.200	2185.653	4957.734	437.477	4385.543	-45.815

3.516. Dibenzo[*c,m*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 222-51-5
Point Group: C_{2v}

Length: 20.17 Å
Width: 9.170 Å
Breadth: 3.884 Å
L/B Ratio: 2.200

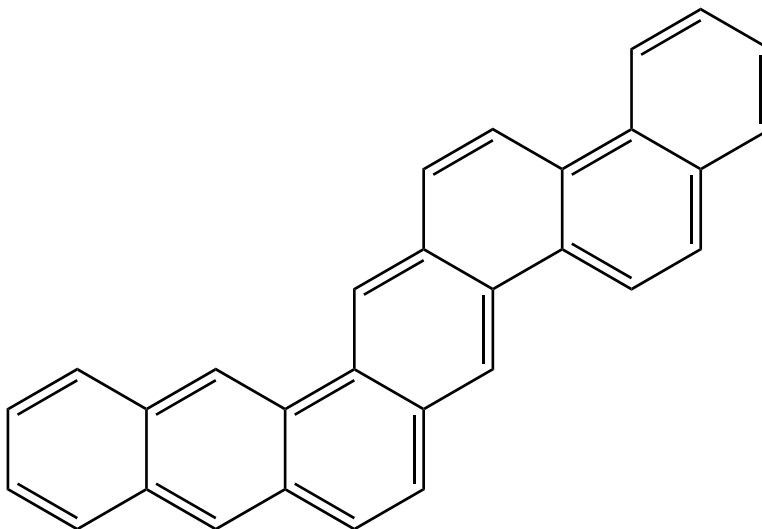
Cartesian coordinates:

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C	7.1051	1.3653	0.0000	C	-2.8131	1.3778	0.0000	H	3.0323	-3.2221	0.0000
C	5.7275	1.3861	0.0000	C	-1.4532	-1.0589	0.0000	H	5.5146	-3.2156	0.0000
C	5.6829	-1.0408	0.0000	C	-2.8514	-1.0483	0.0000	H	3.3623	2.3335	0.0000
C	4.9925	0.1836	0.0000	C	-3.5429	0.1847	0.0000	H	0.9063	-2.0157	0.0000
C	3.5949	-2.2815	0.0000	C	-4.9467	-2.2783	0.0000	H	1.2400	3.5413	0.0000
C	4.9468	-2.2779	0.0000	C	-3.5947	-2.2818	0.0000	H	-1.2403	3.5411	0.0000
C	2.8515	-1.0481	0.0000	C	-5.6829	-1.0412	0.0000	H	-3.3625	2.3333	0.0000
C	3.5428	0.1850	0.0000	C	-4.9926	0.1833	0.0000	H	-0.9061	-2.0158	0.0000
C	2.8130	1.3780	0.0000	C	-5.7276	1.3857	0.0000	H	-5.5143	-3.2160	0.0000
C	1.4533	-1.0588	0.0000	C	-7.1052	1.3647	0.0000	H	-3.0320	-3.2224	0.0000
C	0.7270	0.1307	0.0000	C	-7.7919	0.1415	0.0000	H	-5.1740	2.3372	0.0000
C	1.4198	1.3657	0.0000	C	-7.0923	-1.0460	0.0000	H	-7.6706	2.3023	0.0000
C	0.6745	2.6022	0.0000	H	7.6249	-2.0033	0.0000	H	-8.8868	0.1368	0.0000
C	-0.6747	2.6021	0.0000	H	8.8867	0.1375	0.0000	H	-7.6248	-2.0039	0.0000

Table 3.516: Table of thermodynamic data as a function of temperature for Dibenzo[*c,m*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-56.982	475.806	475.806	∞
100	125.776	369.949	862.467	-49.252	505.496	562.011	-293.559
200	246.292	492.011	646.782	-30.954	489.768	624.799	-163.177
250	316.538	554.458	622.043	-16.896	482.381	659.412	-137.774
298.15	385.119	616.088	616.088	0.000	475.806	694.121	-121.605
300	387.724	618.478	616.096	0.715	475.564	695.474	-121.090
350	456.243	683.444	621.070	21.831	469.509	732.618	-109.335
400	519.837	748.581	632.940	46.256	464.261	770.562	-100.623
450	577.487	813.197	649.386	73.715	459.731	809.127	-93.919
500	629.055	876.763	668.956	103.903	455.821	848.186	-88.608
600	715.628	999.417	713.903	171.309	449.525	927.285	-80.726
700	784.209	1115.081	763.039	246.430	445.015	1007.298	-75.164
800	839.311	1223.524	813.896	327.702	442.080	1087.831	-71.027
900	884.290	1325.064	865.113	413.956	440.517	1168.640	-67.825
1000	921.503	1420.219	915.917	504.302	440.138	1249.573	-65.270
1100	952.617	1509.550	965.865	598.054	440.718	1330.506	-63.179
1200	978.851	1593.595	1014.709	694.663	442.096	1411.330	-61.432
1300	1001.125	1672.848	1062.316	793.692	444.066	1492.027	-59.949
1400	1020.155	1747.754	1108.625	894.781	446.478	1572.558	-58.672
1500	1036.505	1818.709	1153.620	997.634	449.239	1652.907	-57.558
1600	1050.626	1886.065	1197.311	1102.007	452.204	1733.053	-56.577
1700	1062.883	1950.135	1239.725	1207.697	455.288	1812.983	-55.705
1800	1073.574	2011.198	1280.902	1314.532	458.406	1892.802	-54.927
1900	1082.940	2069.499	1320.885	1422.368	461.524	1972.389	-54.224
2000	1091.183	2125.261	1359.720	1531.082	464.579	2051.842	-53.587
2100	1098.466	2178.680	1397.455	1640.572	467.485	2131.129	-53.008
2200	1104.929	2229.932	1434.138	1750.748	470.240	2210.285	-52.478
2300	1110.684	2279.178	1469.815	1861.534	472.837	2289.318	-51.991
2400	1115.828	2326.559	1504.532	1972.865	475.198	2368.189	-51.541
2500	1120.442	2372.204	1538.331	2084.682	477.336	2447.093	-51.128
2600	1124.595	2416.231	1571.255	2196.938	479.209	2525.786	-50.743
2700	1128.343	2458.745	1603.342	2309.588	480.824	2604.492	-50.386
2800	1131.736	2499.843	1634.630	2422.595	482.149	2683.169	-50.054
2900	1134.818	2539.611	1665.155	2535.925	483.153	2761.743	-49.743
3000	1137.623	2578.132	1694.949	2649.549	483.885	2840.317	-49.453
3100	1140.184	2615.476	1724.044	2763.441	484.257	2918.788	-49.180
3200	1142.527	2651.713	1752.470	2877.579	484.316	2997.333	-48.925
3300	1144.676	2686.904	1780.256	2991.940	484.042	3075.924	-48.687
3400	1146.652	2721.106	1807.427	3106.508	483.404	3154.434	-48.461
3500	1148.472	2754.371	1834.009	3221.265	482.406	3232.947	-48.248
3600	1150.151	2786.748	1860.027	3336.198	481.073	3311.590	-48.049
3700	1151.705	2818.283	1885.501	3451.292	479.371	3390.295	-47.861
3800	1153.144	2849.016	1910.454	3566.535	477.270	3468.983	-47.684
3900	1154.480	2878.987	1934.906	3681.917	474.815	3547.675	-47.515
4000	1155.723	2908.232	1958.875	3797.428	471.988	3626.588	-47.357
4100	1156.880	2936.784	1982.379	3913.059	468.749	3705.494	-47.208
4200	1157.959	2964.675	2005.437	4028.801	465.131	3784.474	-47.066
4300	1158.967	2991.934	2028.063	4144.648	461.116	3863.446	-46.931
4400	1159.910	3018.589	2050.273	4260.592	456.715	3942.618	-46.804
4500	1160.794	3044.666	2072.082	4376.628	451.944	4021.956	-46.685
4600	1161.623	3070.188	2093.503	4492.749	446.745	4101.413	-46.572
4700	1162.401	3095.179	2114.551	4608.951	441.135	4180.861	-46.464
4800	1163.133	3119.659	2135.236	4725.228	435.165	4260.549	-46.363
4900	1163.823	3143.649	2155.572	4841.576	428.753	4340.217	-46.266
5000	1164.472	3167.168	2175.570	4957.991	422.003	4420.228	-46.177

3.517. Naphtho[1,2-*c*]pentaphene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-80-3
Point Group: C_s

Length: 20.18 Å
Width: 9.165 Å
Breadth: 3.884 Å
L/B Ratio: 2.202

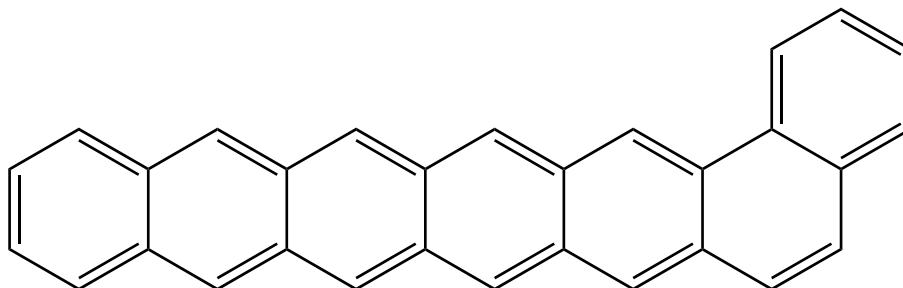
Cartesian coordinates:

C	7.0343	-2.2342	0.0000	C	-0.7484	-0.7898	0.0000	H	7.6725	1.1252	0.0000
C	7.7659	-1.0183	0.0000	C	-1.3993	0.4636	0.0000	H	5.0966	-3.1555	0.0000
C	7.1153	0.1816	0.0000	C	-2.8846	-1.9340	0.0000	H	5.5651	2.3921	0.0000
C	5.6694	-2.2214	0.0000	C	-1.5298	-1.9913	0.0000	H	2.9787	-1.8857	0.0000
C	4.9612	-0.9836	0.0000	C	-3.5740	-0.6778	0.0000	H	3.4950	3.6623	0.0000
C	5.6899	0.2279	0.0000	C	-2.8428	0.5097	0.0000	H	1.0190	3.7419	0.0000
C	4.9951	1.4546	0.0000	C	-3.5304	1.7622	0.0000	H	-1.1352	2.6089	0.0000
C	3.5525	-0.9449	0.0000	C	-4.8883	1.8176	0.0000	H	1.1651	-1.8242	0.0000
C	2.8743	0.2616	0.0000	C	-5.0127	-0.6309	0.0000	H	-3.4938	-2.8510	0.0000
C	3.6113	1.4813	0.0000	C	-5.6633	0.6172	0.0000	H	-1.0064	-2.9542	0.0000
C	2.9000	2.7415	0.0000	C	-7.0784	0.6699	0.0000	H	-2.9238	2.6810	0.0000
C	1.5539	2.7850	0.0000	C	-7.8153	-0.4879	0.0000	H	-5.4121	2.7803	0.0000
C	1.4177	0.3122	0.0000	C	-7.1679	-1.7395	0.0000	H	-7.5738	1.6475	0.0000
C	0.7647	1.5726	0.0000	C	-5.7976	-1.8101	0.0000	H	-8.9094	-0.4499	0.0000
C	-0.6217	1.6339	0.0000	H	7.5833	-3.1816	0.0000	H	-7.7694	-2.6544	0.0000
C	0.6546	-0.8474	0.0000	H	8.8600	-1.0597	0.0000	H	-5.2806	-2.7818	0.0000

Table 3.517: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*c*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.088	486.533	486.533	∞
100	126.057	376.867	870.099	-49.323	516.152	571.975	-298.763
200	246.674	499.170	654.121	-30.990	500.459	634.058	-165.596
250	316.912	561.702	629.355	-16.913	493.092	668.311	-139.633
298.15	385.449	623.395	623.395	0.000	486.533	702.669	-123.102
300	388.051	625.787	623.402	0.715	486.291	704.009	-122.576
350	456.503	690.798	628.380	21.846	480.251	740.787	-110.554
400	520.026	755.965	640.258	46.283	475.015	778.362	-101.642
450	577.614	820.600	656.712	73.749	470.492	816.558	-94.782
500	629.131	884.176	676.291	103.943	466.588	855.246	-89.345
600	715.631	1006.838	721.251	171.352	460.296	933.603	-81.276
700	784.168	1122.499	770.397	246.471	455.783	1012.875	-75.580
800	839.243	1230.934	821.261	327.738	452.843	1092.665	-71.342
900	884.208	1332.465	872.483	413.984	451.273	1172.734	-68.062
1000	921.413	1427.611	923.289	504.322	450.885	1252.928	-65.445
1100	952.523	1516.933	973.239	598.064	451.455	1333.122	-63.303
1200	978.757	1600.970	1022.083	694.664	452.824	1413.208	-61.514
1300	1001.033	1680.216	1069.690	793.683	454.784	1493.168	-59.995
1400	1020.066	1755.115	1115.999	894.763	457.188	1572.963	-58.687
1500	1036.420	1826.064	1160.992	997.607	459.940	1652.576	-57.547
1600	1050.545	1893.415	1204.682	1101.973	462.896	1731.987	-56.542
1700	1062.807	1957.480	1247.095	1207.654	465.972	1811.182	-55.650
1800	1073.502	2018.538	1288.270	1314.482	469.084	1890.266	-54.853
1900	1082.872	2076.836	1328.251	1422.311	472.194	1969.119	-54.134
2000	1091.119	2132.594	1367.085	1531.019	475.243	2047.839	-53.483
2100	1098.406	2186.010	1404.818	1640.502	478.142	2126.393	-52.890
2200	1104.872	2237.260	1441.500	1750.673	480.892	2204.816	-52.348
2300	1110.631	2286.503	1477.175	1861.453	483.483	2283.116	-51.850
2400	1115.778	2333.882	1511.891	1972.778	485.839	2361.255	-51.390
2500	1120.395	2379.525	1545.689	2084.591	487.972	2439.427	-50.968
2600	1124.550	2423.550	1578.611	2196.842	489.841	2517.388	-50.574
2700	1128.301	2466.063	1610.697	2309.488	491.451	2595.362	-50.209
2800	1131.697	2507.159	1641.984	2422.491	492.772	2673.307	-49.870
2900	1134.781	2546.926	1672.506	2535.817	493.773	2751.150	-49.553
3000	1137.588	2585.445	1702.299	2649.437	494.500	2828.992	-49.256
3100	1140.151	2622.789	1731.393	2763.326	494.869	2906.732	-48.977
3200	1142.496	2659.025	1759.818	2877.460	494.925	2984.546	-48.717
3300	1144.646	2694.214	1787.603	2991.819	494.648	3062.406	-48.473
3400	1146.623	2728.415	1814.773	3106.384	494.007	3140.185	-48.242
3500	1148.444	2761.680	1841.354	3221.138	493.006	3217.967	-48.025
3600	1150.125	2794.056	1867.371	3336.068	491.671	3295.879	-47.821
3700	1151.680	2825.590	1892.844	3451.159	489.966	3373.854	-47.629
3800	1153.121	2856.323	1917.796	3566.400	487.862	3451.810	-47.447
3900	1154.458	2886.293	1942.247	3681.780	485.405	3529.772	-47.275
4000	1155.701	2915.537	1966.215	3797.289	482.576	3607.955	-47.114
4100	1156.859	2944.089	1989.719	3912.917	479.335	3686.130	-46.961
4200	1157.939	2971.979	2012.775	4028.658	475.715	3764.380	-46.816
4300	1158.948	2999.238	2035.400	4144.503	471.698	3842.621	-46.678
4400	1159.892	3025.893	2057.610	4260.445	467.295	3921.062	-46.548
4500	1160.776	3051.969	2079.418	4376.479	462.522	3999.671	-46.426
4600	1161.606	3077.491	2100.839	4492.599	457.322	4078.397	-46.311
4700	1162.385	3102.481	2121.885	4608.799	451.710	4157.115	-46.200
4800	1163.118	3126.961	2142.570	4725.074	445.738	4236.073	-46.097
4900	1163.808	3150.951	2162.906	4841.421	439.325	4315.011	-45.998
5000	1164.458	3174.469	2182.902	4957.834	432.573	4394.291	-45.906

3.518. Benzo[*a*]hexacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 240-04-0
Point Group: C_s

Length: 20.72 Å
Width: 9.208 Å
Breadth: 3.885 Å
L/B Ratio: 2.250

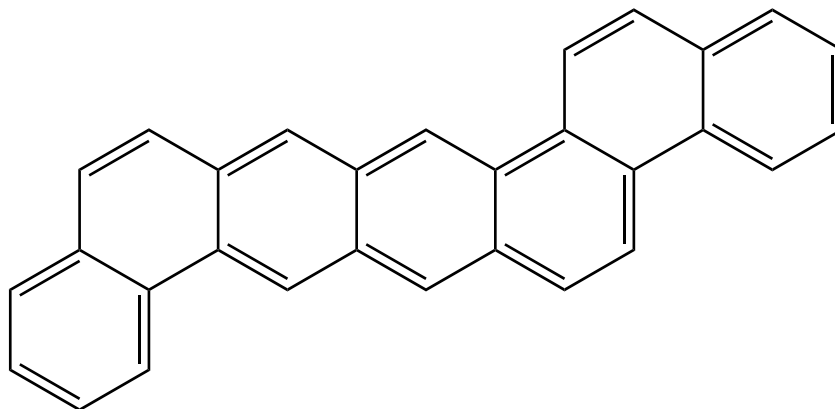
Cartesian coordinates:

C	-8.2572	1.1563	0.0000	C	1.4305	0.2323	0.0000	H	-7.3947	-2.1620	0.0000
C	-8.3934	-0.2720	0.0000	C	1.2947	-1.1951	0.0000	H	-6.9195	2.8236	0.0000
C	-7.3008	-1.0701	0.0000	C	2.4802	-1.9996	0.0000	H	-4.9506	-2.3955	0.0000
C	-7.0336	1.7336	0.0000	C	2.7458	0.7984	0.0000	H	-4.4753	2.5912	0.0000
C	-5.8364	0.9273	0.0000	C	3.8624	0.0088	0.0000	H	-2.5115	-2.6259	0.0000
C	-5.9728	-0.5044	0.0000	C	3.7227	-1.4283	0.0000	H	-2.0367	2.3567	0.0000
C	-4.8533	-1.3027	0.0000	C	4.9171	-2.2498	0.0000	H	-0.0734	-2.8595	0.0000
C	-4.5862	1.4997	0.0000	C	6.1459	-1.7013	0.0000	H	0.4021	2.1253	0.0000
C	-3.4135	0.6924	0.0000	C	5.2043	0.5819	0.0000	H	2.3676	-3.0911	0.0000
C	-3.5492	-0.7314	0.0000	C	6.3256	-0.2649	0.0000	H	2.8537	1.8953	0.0000
C	-2.4088	-1.5335	0.0000	C	7.6154	0.2879	0.0000	H	4.7842	-3.3381	0.0000
C	-2.1421	1.2646	0.0000	C	7.7864	1.6610	0.0000	H	7.0457	-2.3274	0.0000
C	-0.9918	0.4607	0.0000	C	6.6736	2.5056	0.0000	H	8.4870	-0.3765	0.0000
C	-1.1273	-0.9614	0.0000	C	5.3975	1.9720	0.0000	H	8.7941	2.0891	0.0000
C	0.0353	-1.7677	0.0000	H	-9.1678	1.7642	0.0000	H	6.8141	3.5914	0.0000
C	0.3023	1.0328	0.0000	H	-9.4024	-0.6970	0.0000	H	4.5126	2.6270	0.0000

Table 3.518: Table of thermodynamic data as a function of temperature for Benzo[*a*]hexacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-57.768	551.866	551.866	∞
100	127.302	385.836	883.971	-49.813	580.994	635.921	-332.164
200	249.187	509.332	665.837	-31.301	565.481	697.048	-182.046
250	320.129	572.504	640.824	-17.080	558.258	730.777	-152.684
298.15	389.117	634.806	634.806	0.000	551.866	764.600	-133.952
300	391.731	637.221	634.813	0.722	551.631	765.918	-133.355
350	460.395	702.818	639.837	22.043	545.781	802.109	-119.706
400	523.939	768.507	651.818	46.676	540.740	839.071	-109.569
450	581.426	833.599	668.408	74.336	536.411	876.627	-101.754
500	632.775	897.568	688.137	104.716	532.693	914.656	-95.551
600	718.867	1020.858	733.410	172.469	526.745	991.640	-86.328
700	787.005	1136.988	782.857	247.891	522.536	1069.485	-79.804
800	841.731	1245.778	833.998	329.424	519.862	1147.809	-74.943
900	886.400	1347.584	885.470	415.903	518.525	1226.379	-71.176
1000	923.356	1442.948	936.500	506.448	518.343	1305.049	-68.167
1100	954.255	1532.445	986.652	600.373	519.098	1383.701	-65.705
1200	980.307	1616.625	1035.677	697.138	520.630	1462.228	-63.648
1300	1002.428	1695.989	1083.447	796.304	522.737	1540.616	-61.901
1400	1021.326	1770.986	1129.903	897.516	525.273	1618.829	-60.398
1500	1037.561	1842.018	1175.031	1000.480	528.146	1696.850	-59.088
1600	1051.583	1909.439	1218.842	1104.954	531.211	1774.662	-57.936
1700	1063.754	1973.564	1261.367	1210.735	534.386	1852.252	-56.912
1800	1074.368	2034.674	1302.645	1317.653	537.588	1929.726	-55.998
1900	1083.668	2093.017	1342.719	1425.565	540.782	2006.963	-55.174
2000	1091.851	2148.814	1381.639	1534.350	543.906	2084.062	-54.429
2100	1099.082	2202.264	1419.453	1643.904	546.876	2160.992	-53.751
2200	1105.498	2253.545	1456.209	1754.139	549.691	2237.789	-53.131
2300	1111.211	2302.814	1491.954	1864.980	552.342	2314.459	-52.562
2400	1116.317	2350.217	1526.733	1976.361	554.755	2390.966	-52.037
2500	1120.898	2395.882	1560.592	2088.226	556.939	2467.502	-51.555
2600	1125.019	2439.926	1593.570	2200.525	558.857	2543.827	-51.105
2700	1128.740	2482.456	1625.709	2313.216	560.512	2620.162	-50.689
2800	1132.108	2523.567	1657.045	2426.261	561.876	2696.467	-50.302
2900	1135.167	2563.348	1687.615	2539.628	562.916	2772.669	-49.940
3000	1137.951	2601.880	1717.451	2653.286	563.681	2848.868	-49.602
3100	1140.493	2639.235	1746.587	2767.210	564.085	2924.964	-49.284
3200	1142.819	2675.482	1775.051	2881.377	564.175	3001.132	-48.987
3300	1144.951	2710.681	1802.873	2995.767	563.929	3077.347	-48.709
3400	1146.912	2744.891	1830.079	3110.362	563.317	3153.478	-48.446
3500	1148.718	2778.163	1856.694	3225.144	562.345	3229.613	-48.198
3600	1150.385	2810.548	1882.742	3340.101	561.036	3305.876	-47.966
3700	1151.927	2842.088	1908.246	3455.217	559.357	3382.201	-47.747
3800	1153.356	2872.827	1933.227	3570.482	557.277	3458.507	-47.540
3900	1154.681	2902.804	1957.705	3685.885	554.842	3534.818	-47.343
4000	1155.914	2932.053	1981.700	3801.415	552.035	3611.349	-47.158
4100	1157.063	2960.610	2005.229	3917.065	548.816	3687.873	-46.983
4200	1158.134	2988.506	2028.309	4032.825	545.215	3764.470	-46.817
4300	1159.134	3015.769	2050.957	4148.689	541.217	3841.059	-46.659
4400	1160.070	3042.428	2073.189	4264.650	536.833	3917.847	-46.510
4500	1160.947	3068.508	2095.019	4380.701	532.077	3994.801	-46.369
4600	1161.769	3094.033	2116.460	4496.838	526.893	4071.873	-46.237
4700	1162.542	3119.027	2137.526	4613.053	521.297	4148.937	-46.109
4800	1163.268	3143.510	2158.230	4729.344	515.341	4226.241	-45.990
4900	1163.952	3167.503	2178.583	4845.706	508.942	4303.523	-45.875
5000	1164.597	3191.024	2198.598	4962.134	502.205	4381.149	-45.769

3.519. Benzo[*a*]naphtho[2,1-*j*]naphthacene



Other names: Phenanthro[3,2-*b*]chrysene

Formula: C₃₀H₁₈

Mass: 378.464 g/mol

CAS Number: 112498-97-2

Point Group: C_s

Length: 20.16 Å

Width: 9.018 Å

Breadth: 3.884 Å

L/B Ratio: 2.236

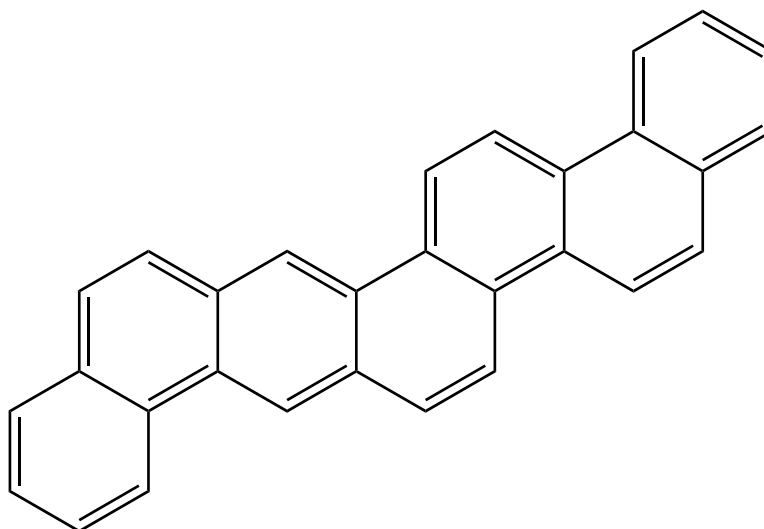
Cartesian coordinates:

C	7.3772	-0.3870	0.0000	C	-1.4380	-0.0450	0.0000	H	7.1796	3.0059	0.0000
C	7.7902	0.9314	0.0000	C	-1.0428	1.3274	0.0000	H	4.7419	2.4701	0.0000
C	6.8453	1.9633	0.0000	C	-2.0589	2.3493	0.0000	H	3.9333	-3.4405	0.0000
C	5.4961	1.6681	0.0000	C	-3.3701	2.0246	0.0000	H	6.3429	-2.8587	0.0000
C	6.0072	-0.7011	0.0000	C	-2.8540	-0.3683	0.0000	H	2.9784	2.0507	0.0000
C	5.0560	0.3331	0.0000	C	-3.8012	0.6511	0.0000	H	1.5994	-2.7583	0.0000
C	4.2622	-2.3948	0.0000	C	-4.6044	-2.0495	0.0000	H	0.6029	2.7194	0.0000
C	5.5725	-2.0788	0.0000	C	-3.2817	-1.7288	0.0000	H	-0.7684	-2.0900	0.0000
C	3.2430	-1.3685	0.0000	C	-5.5967	-1.0250	0.0000	H	-1.7369	3.3971	0.0000
C	3.6369	0.0077	0.0000	C	-5.2010	0.3265	0.0000	H	-4.1505	2.8011	0.0000
C	2.6713	0.9923	0.0000	C	-6.2026	1.3305	0.0000	H	-4.9285	-3.0965	0.0000
C	1.9053	-1.7047	0.0000	C	-7.5316	0.9942	0.0000	H	-2.5084	-2.5124	0.0000
C	0.9058	-0.7006	0.0000	C	-7.9233	-0.3608	0.0000	H	-5.8854	2.3844	0.0000
C	1.2937	0.6641	0.0000	C	-6.9760	-1.3522	0.0000	H	-8.3004	1.7738	0.0000
C	0.3003	1.6648	0.0000	H	8.1150	-1.1975	0.0000	H	-8.9893	-0.6103	0.0000
C	-0.4649	-1.0307	0.0000	H	8.8579	1.1736	0.0000	H	-7.2709	-2.4077	0.0000

Table 3.519: Table of thermodynamic data as a function of temperature for Benzo[*a*]naphtho[2,1-*j*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298 \text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	Δ _f <i>H</i> ^o	Δ _f <i>G</i> ^o	log <i>K</i> _f
0	0.0	0.0	∞	-57.318	495.452	495.452	∞
100	126.702	380.871	875.286	-49.442	524.953	580.376	-303.151
200	247.239	503.532	658.818	-31.057	509.311	642.038	-167.680
250	317.606	566.204	633.999	-16.949	501.976	676.069	-141.254
298.15	386.219	628.027	628.027	0.000	495.452	710.208	-124.423
300	388.824	630.424	628.034	0.717	495.212	711.539	-123.887
350	457.302	695.556	633.021	21.887	489.211	748.082	-111.643
400	520.815	760.829	644.920	46.364	484.015	785.417	-102.563
450	578.370	825.556	661.403	73.869	479.531	823.366	-95.572
500	629.841	889.209	681.011	104.099	475.663	861.805	-90.030
600	716.237	1011.991	726.035	171.574	469.437	939.652	-81.802
700	784.675	1127.738	775.240	246.748	464.980	1018.404	-75.993
800	839.664	1236.235	826.158	328.062	462.086	1097.668	-71.669
900	884.557	1337.811	877.427	414.346	460.554	1177.204	-68.322
1000	921.704	1432.991	928.275	504.716	460.198	1256.861	-65.650
1100	952.768	1522.338	978.262	598.484	460.796	1336.516	-63.465
1200	978.963	1606.395	1027.139	695.107	462.186	1416.061	-61.638
1300	1001.210	1685.656	1074.775	794.145	464.166	1495.477	-60.088
1400	1020.218	1760.567	1121.109	895.241	466.586	1574.727	-58.753
1500	1036.551	1831.526	1166.126	998.100	469.352	1653.794	-57.589
1600	1050.660	1898.885	1209.836	1102.478	472.321	1732.659	-56.564
1700	1062.908	1962.957	1252.268	1208.170	475.407	1811.307	-55.654
1800	1073.591	2024.020	1293.461	1315.007	478.528	1889.843	-54.841
1900	1082.952	2082.322	1333.457	1422.844	481.648	1968.148	-54.107
2000	1091.190	2138.084	1372.304	1531.560	484.703	2046.318	-53.443
2100	1098.471	2191.504	1410.051	1641.050	487.610	2124.323	-52.839
2200	1104.930	2242.756	1446.744	1751.227	490.365	2202.197	-52.286
2300	1110.684	2292.002	1482.431	1862.013	492.962	2279.948	-51.778
2400	1115.827	2339.383	1517.156	1973.343	495.324	2357.537	-51.309
2500	1120.440	2385.028	1550.964	2085.161	497.461	2435.158	-50.879
2600	1124.591	2429.055	1583.895	2197.416	499.334	2512.569	-50.477
2700	1128.339	2471.569	1615.989	2310.065	500.948	2589.992	-50.105
2800	1131.732	2512.666	1647.284	2423.072	502.273	2667.386	-49.760
2900	1134.813	2552.435	1677.814	2536.401	503.277	2744.678	-49.436
3000	1137.618	2590.955	1707.613	2650.025	504.007	2821.970	-49.134
3100	1140.179	2628.299	1736.713	2763.917	504.379	2899.159	-48.849
3200	1142.522	2664.536	1765.144	2878.054	504.438	2976.421	-48.584
3300	1144.671	2699.727	1792.934	2992.415	504.163	3053.730	-48.336
3400	1146.646	2733.928	1820.110	3106.982	503.524	3130.958	-48.100
3500	1148.466	2767.193	1846.697	3221.739	502.526	3208.189	-47.879
3600	1150.146	2799.571	1872.718	3336.671	501.193	3285.549	-47.671
3700	1151.700	2831.105	1898.196	3451.764	499.490	3362.972	-47.476
3800	1153.139	2861.838	1923.152	3567.007	497.388	3440.377	-47.290
3900	1154.475	2891.809	1947.607	3682.388	494.932	3517.788	-47.115
4000	1155.718	2921.054	1971.579	3797.899	492.105	3595.419	-46.950
4100	1156.875	2949.606	1995.086	3913.529	488.866	3673.043	-46.794
4200	1157.954	2977.497	2018.146	4029.271	485.247	3750.741	-46.646
4300	1158.962	3004.756	2040.775	4145.117	481.232	3828.430	-46.505
4400	1159.906	3031.411	2062.988	4261.061	476.831	3906.320	-46.373
4500	1160.789	3057.487	2084.799	4377.096	472.059	3984.376	-46.248
4600	1161.618	3083.009	2106.223	4493.217	466.860	4062.550	-46.131
4700	1162.397	3108.000	2127.272	4609.418	461.249	4140.716	-46.018
4800	1163.129	3132.480	2147.960	4725.695	455.278	4219.123	-45.912
4900	1163.818	3156.470	2168.298	4842.043	448.866	4297.509	-45.811
5000	1164.468	3179.989	2188.297	4958.457	442.116	4376.238	-45.717

3.520. Naphtho[2,1-*b*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 115747-81-4
Point Group: C_s

Length: 20.07 Å
Width: 8.916 Å
Breadth: 3.884 Å
L/B Ratio: 2.251

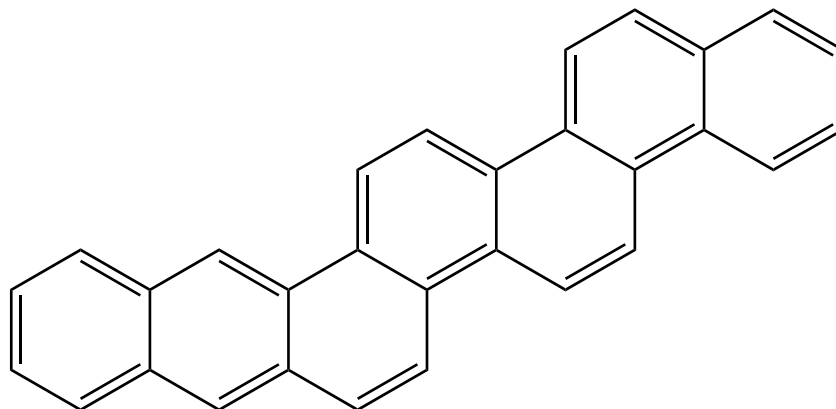
Cartesian coordinates:

C	7.1678	-0.8731	0.0000	C	-0.7111	-0.2248	0.0000	H	7.5195	2.5068	0.0000
C	7.7863	0.3595	0.0000	C	-1.4865	0.9390	0.0000	H	5.0261	2.3729	0.0000
C	7.0191	1.5330	0.0000	C	-2.7145	-1.5859	0.0000	H	3.2660	-3.3207	0.0000
C	5.6424	1.4607	0.0000	C	-1.3528	-1.4914	0.0000	H	5.7408	-3.1448	0.0000
C	5.7621	-0.9629	0.0000	C	-3.5245	-0.4196	0.0000	H	3.2175	2.2457	0.0000
C	4.9909	0.2121	0.0000	C	-2.9148	0.8416	0.0000	H	1.0670	-2.2631	0.0000
C	3.7630	-2.3437	0.0000	C	-3.7374	2.0165	0.0000	H	1.0075	3.3016	0.0000
C	5.1105	-2.2480	0.0000	C	-5.0903	1.9290	0.0000	H	-1.4686	3.1179	0.0000
C	2.9348	-1.1635	0.0000	C	-4.9648	-0.5209	0.0000	H	-3.2151	-2.5664	0.0000
C	3.5429	0.1167	0.0000	C	-5.7401	0.6522	0.0000	H	-0.7225	-2.3940	0.0000
C	2.7372	1.2537	0.0000	C	-7.1505	0.5597	0.0000	H	-3.2345	2.9955	0.0000
C	1.5454	-1.2704	0.0000	C	-7.7648	-0.6700	0.0000	H	-5.7129	2.8311	0.0000
C	0.7340	-0.1305	0.0000	C	-6.9928	-1.8458	0.0000	H	-7.7454	1.4801	0.0000
C	1.3430	1.1467	0.0000	C	-5.6205	-1.7734	0.0000	H	-8.8572	-0.7435	0.0000
C	0.5163	2.3218	0.0000	H	7.7640	-1.7927	0.0000	H	-7.4946	-2.8189	0.0000
C	-0.8330	2.2193	0.0000	H	8.8790	0.4281	0.0000	H	-5.0053	-2.6861	0.0000

Table 3.520: Table of thermodynamic data as a function of temperature for Naphtho[2,1-*b*]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-57.118	480.183	480.183	∞
100	126.702	379.171	871.862	-49.269	509.856	565.449	-295.354
200	246.342	501.583	656.213	-30.926	494.173	627.290	-163.828
250	316.241	564.003	631.501	-16.874	486.781	661.425	-138.194
298.15	384.522	625.555	625.555	0.000	480.183	695.676	-121.877
300	387.117	627.941	625.562	0.714	479.940	697.011	-121.358
350	455.398	692.794	630.528	21.793	473.848	733.685	-109.494
400	518.834	757.807	642.377	46.172	468.554	771.165	-100.702
450	576.394	822.300	658.793	73.578	463.971	809.272	-93.936
500	627.922	885.748	678.326	103.711	460.006	847.879	-88.575
600	714.496	1008.194	723.191	171.002	453.596	926.089	-80.622
700	783.127	1123.688	772.241	246.012	448.975	1005.234	-75.010
800	838.291	1231.990	823.015	327.180	445.935	1084.913	-70.836
900	883.336	1333.413	874.153	413.334	444.273	1164.882	-67.607
1000	920.613	1428.471	924.882	503.589	443.802	1244.985	-65.030
1100	951.789	1517.720	974.762	597.254	444.296	1325.097	-62.922
1200	978.082	1601.695	1023.542	693.784	445.594	1405.108	-61.161
1300	1000.413	1680.889	1071.090	792.739	447.490	1484.997	-59.667
1400	1019.496	1755.745	1117.346	893.759	449.834	1564.727	-58.379
1500	1035.894	1826.656	1162.290	996.548	452.532	1644.279	-57.258
1600	1050.061	1893.974	1205.934	1100.863	455.437	1723.633	-56.270
1700	1062.359	1958.011	1248.306	1206.498	458.467	1802.774	-55.391
1800	1073.088	2019.044	1289.443	1313.283	461.535	1881.806	-54.607
1900	1082.489	2077.321	1329.388	1421.072	464.606	1960.609	-53.900
2000	1090.764	2133.060	1368.188	1529.743	467.617	2039.281	-53.259
2100	1098.076	2186.459	1405.891	1639.192	470.483	2117.790	-52.676
2200	1104.565	2237.694	1442.544	1749.331	473.200	2196.169	-52.143
2300	1110.344	2286.924	1478.193	1860.082	475.762	2274.426	-51.653
2400	1115.511	2334.291	1512.883	1971.379	478.090	2352.524	-51.200
2500	1120.145	2379.924	1546.658	2083.166	480.197	2430.655	-50.785
2600	1124.316	2423.940	1579.558	2195.393	482.042	2508.576	-50.397
2700	1128.081	2466.444	1611.623	2308.016	483.629	2586.512	-50.038
2800	1131.490	2507.532	1642.890	2420.997	484.929	2664.419	-49.704
2900	1134.586	2547.292	1673.394	2534.303	485.910	2742.225	-49.392
3000	1137.404	2585.805	1703.170	2647.905	486.618	2820.031	-49.100
3100	1139.977	2623.142	1732.247	2761.776	486.969	2897.735	-48.825
3200	1142.332	2659.373	1760.656	2875.893	487.008	2975.514	-48.569
3300	1144.491	2694.558	1788.426	2990.236	486.715	3053.340	-48.329
3400	1146.476	2728.754	1815.582	3104.786	486.059	3131.084	-48.102
3500	1148.305	2762.015	1842.150	3219.526	485.044	3208.833	-47.888
3600	1149.993	2794.387	1868.153	3334.442	483.695	3286.712	-47.688
3700	1151.554	2825.917	1893.615	3449.520	481.977	3364.653	-47.499
3800	1153.000	2856.647	1918.555	3564.749	479.861	3442.577	-47.321
3900	1154.343	2886.614	1942.994	3680.117	477.392	3520.507	-47.151
4000	1155.592	2915.856	1966.952	3795.614	474.552	3598.657	-46.993
4100	1156.755	2944.405	1990.445	3911.232	471.301	3676.801	-46.842
4200	1157.839	2972.293	2013.492	4026.963	467.670	3755.020	-46.700
4300	1158.852	2999.549	2036.108	4142.798	463.643	3833.229	-46.564
4400	1159.800	3026.202	2058.308	4258.731	459.231	3911.640	-46.436
4500	1160.688	3052.276	2080.108	4374.756	454.449	3990.217	-46.316
4600	1161.522	3077.796	2101.520	4490.867	449.240	4068.913	-46.203
4700	1162.304	3102.784	2122.559	4607.059	443.620	4147.600	-46.094
4800	1163.040	3127.262	2143.236	4723.326	437.640	4226.529	-45.993
4900	1163.733	3151.251	2163.564	4839.665	431.219	4305.436	-45.896
5000	1164.386	3174.768	2183.553	4956.071	424.461	4384.687	-45.806

3.521. Dibenzo[*b,m*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 82628-46-4
Point Group: C_s

Length: 20.32 Å
Width: 8.921 Å
Breadth: 3.887 Å
L/B Ratio: 2.278

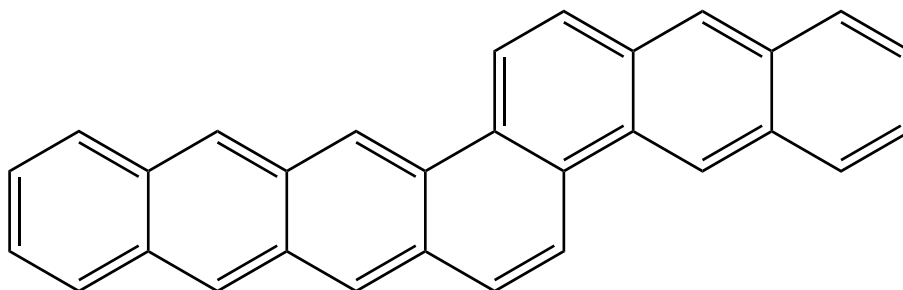
Cartesian coordinates:

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C	7.9185	-0.4118	0.0000	C	-0.8280	0.7807	0.0000	H	5.6381	-2.9621	0.0000
C	7.0814	0.6632	0.0000	C	-1.7209	1.8942	0.0000	H	5.1860	2.5878	0.0000
C	6.0498	-1.9466	0.0000	C	-3.0687	1.7124	0.0000	H	3.3449	-2.0600	0.0000
C	5.1433	-0.8413	0.0000	C	-2.7853	-0.7083	0.0000	H	2.9237	3.4935	0.0000
C	5.6642	0.4763	0.0000	C	-3.6325	0.4027	0.0000	H	0.4665	3.1451	0.0000
C	4.7820	1.5678	0.0000	C	-4.6968	-2.2092	0.0000	H	-0.9016	-2.6426	0.0000
C	3.7539	-1.0368	0.0000	C	-3.3522	-2.0230	0.0000	H	1.5681	-2.3059	0.0000
C	2.8794	0.0441	0.0000	C	-5.5873	-1.0893	0.0000	H	-1.2891	2.9065	0.0000
C	3.4067	1.3656	0.0000	C	-5.0618	0.2155	0.0000	H	-3.7583	2.5706	0.0000
C	2.4988	2.4831	0.0000	C	-5.9557	1.3126	0.0000	H	-5.1253	-3.2180	0.0000
C	1.1611	2.2913	0.0000	C	-7.3137	1.1093	0.0000	H	-2.6625	-2.8808	0.0000
C	1.4401	-0.1398	0.0000	C	-7.8358	-0.1982	0.0000	H	-5.5348	2.3296	0.0000
C	0.5930	0.9687	0.0000	C	-6.9892	-1.2798	0.0000	H	-8.0007	1.9619	0.0000
C	-0.4709	-1.6297	0.0000	H	8.0948	-2.5770	0.0000	H	-8.9210	-0.3431	0.0000
C	0.8803	-1.4462	0.0000	H	9.0048	-0.2748	0.0000	H	-7.3877	-2.3007	0.0000

Table 3.521: Table of thermodynamic data as a function of temperature for Dibenzo[*b,m*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.693	490.771	490.771	∞
100	128.290	388.802	884.789	-49.599	520.114	574.744	-300.209
200	248.017	512.322	667.798	-31.095	504.591	635.561	-165.988
250	317.976	575.123	642.956	-16.958	497.284	669.149	-139.808
298.15	386.256	636.981	636.981	0.000	490.771	702.856	-123.135
300	388.849	639.378	636.988	0.717	490.531	704.171	-122.604
350	457.074	704.495	641.975	21.882	484.524	740.266	-110.476
400	520.417	769.725	653.870	46.342	479.312	777.155	-101.484
450	577.867	834.398	670.343	73.825	474.805	814.661	-94.561
500	629.278	897.996	689.939	104.028	470.911	852.659	-89.075
600	715.628	1020.669	734.930	171.444	464.625	929.633	-80.930
700	784.064	1136.322	784.097	246.557	460.107	1007.522	-75.181
800	839.067	1244.738	834.976	327.810	457.153	1085.932	-70.903
900	883.982	1346.245	886.206	414.035	455.562	1164.621	-67.591
1000	921.155	1441.366	937.017	504.349	455.150	1243.438	-64.949
1100	952.247	1530.662	986.968	598.064	455.694	1322.258	-62.788
1200	978.473	1614.675	1035.811	694.637	457.034	1400.973	-60.981
1300	1000.749	1693.898	1083.415	793.627	458.966	1479.563	-59.448
1400	1019.787	1768.776	1129.720	894.679	461.341	1557.991	-58.128
1500	1036.149	1839.706	1174.709	997.496	464.066	1636.238	-56.978
1600	1050.285	1907.040	1218.393	1101.834	466.996	1714.286	-55.965
1700	1062.558	1971.090	1260.801	1207.491	470.046	1792.120	-55.064
1800	1073.265	2032.134	1301.971	1314.294	473.133	1869.844	-54.260
1900	1082.648	2090.419	1341.946	1422.100	476.221	1947.338	-53.535
2000	1090.907	2146.166	1380.773	1530.786	479.248	2024.699	-52.879
2100	1098.206	2199.572	1418.501	1640.249	482.127	2101.897	-52.281
2200	1104.683	2250.813	1455.177	1750.400	484.856	2178.965	-51.734
2300	1110.452	2300.048	1490.847	1861.162	487.430	2255.910	-51.232
2400	1115.610	2347.419	1525.557	1972.470	489.769	2332.695	-50.769
2500	1120.236	2393.056	1559.349	2084.266	491.885	2409.512	-50.343
2600	1124.400	2437.075	1592.267	2196.502	493.738	2486.121	-49.946
2700	1128.159	2479.582	1624.348	2309.133	495.333	2562.743	-49.578
2800	1131.562	2520.673	1655.629	2422.122	496.641	2639.336	-49.236
2900	1134.653	2560.436	1686.148	2535.435	497.628	2715.828	-48.916
3000	1137.467	2598.950	1715.936	2649.043	498.344	2792.320	-48.618
3100	1140.036	2636.290	1745.026	2762.920	498.701	2868.709	-48.336
3200	1142.387	2672.523	1773.447	2877.043	498.746	2945.173	-48.074
3300	1144.543	2707.709	1801.227	2991.391	498.458	3021.683	-47.828
3400	1146.525	2741.907	1828.394	3105.946	497.806	3098.113	-47.596
3500	1148.351	2775.169	1854.971	3220.691	496.796	3174.546	-47.377
3600	1150.036	2807.543	1880.984	3335.611	495.452	3251.109	-47.171
3700	1151.595	2839.074	1906.454	3450.694	493.738	3327.735	-46.978
3800	1153.039	2869.804	1931.403	3565.926	491.626	3404.344	-46.795
3900	1154.380	2899.773	1955.850	3681.298	489.161	3480.957	-46.621
4000	1155.627	2929.015	1979.815	3796.799	486.324	3557.792	-46.459
4100	1156.788	2957.565	2003.316	3912.421	483.076	3634.620	-46.305
4200	1157.871	2985.454	2026.369	4028.154	479.449	3711.522	-46.159
4300	1158.883	3012.711	2048.992	4143.992	475.425	3788.416	-46.019
4400	1159.829	3039.364	2071.199	4259.928	471.016	3865.510	-45.888
4500	1160.716	3065.439	2093.004	4375.956	466.237	3942.771	-45.766
4600	1161.548	3090.959	2114.422	4492.070	461.031	4020.150	-45.649
4700	1162.329	3115.948	2135.466	4608.264	455.413	4097.522	-45.538
4800	1163.064	3140.427	2156.149	4724.534	449.436	4175.133	-45.434
4900	1163.756	3164.416	2176.482	4840.876	443.017	4252.724	-45.334
5000	1164.408	3187.933	2196.477	4957.284	436.261	4330.659	-45.241

3.522. Anthra[2,1-*a*]naphthacene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 214-16-4
Point Group: C_s

Length: 20.78 Å
Width: 9.024 Å
Breadth: 3.884 Å
L/B Ratio: 2.303

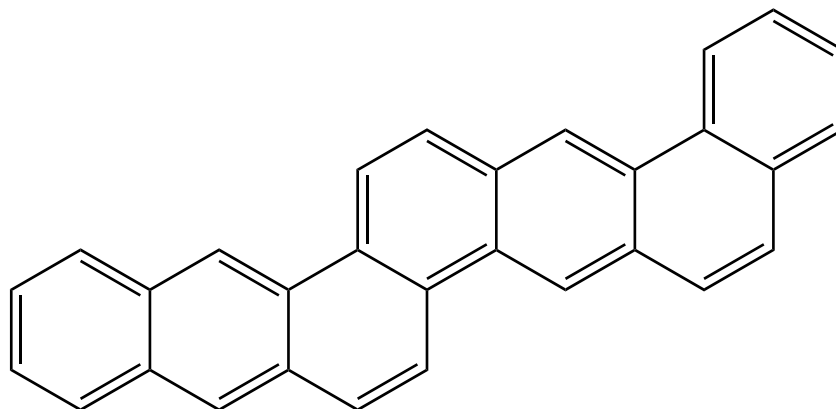
Cartesian coordinates:

C	7.9135	-1.2983	0.0000	C	-0.6360	-0.3905	0.0000	H	7.3565	2.0813	0.0000
C	8.1802	0.1061	0.0000	C	-1.6663	0.5356	0.0000	H	6.4231	-2.8342	0.0000
C	7.1621	1.0028	0.0000	C	-2.2198	-2.2337	0.0000	H	4.9432	2.5402	0.0000
C	6.6375	-1.7594	0.0000	C	-0.9392	-1.7922	0.0000	H	4.0098	-2.3766	0.0000
C	5.5280	-0.8448	0.0000	C	-3.3158	-1.3060	0.0000	H	2.5305	2.9935	0.0000
C	5.7945	0.5585	0.0000	C	-3.0429	0.0902	0.0000	H	1.5959	-1.9207	0.0000
C	4.7420	1.4618	0.0000	C	-4.1079	0.9898	0.0000	H	0.1390	3.4583	0.0000
C	4.2177	-1.2995	0.0000	C	-4.6331	-1.7607	0.0000	H	-2.2093	2.6457	0.0000
C	3.1429	-0.3889	0.0000	C	-5.7000	-0.8544	0.0000	H	-2.4464	-3.3061	0.0000
C	3.4084	1.0083	0.0000	C	-5.4329	0.5390	0.0000	H	-0.0945	-2.4983	0.0000
C	2.3225	1.9162	0.0000	C	-6.5317	1.4563	0.0000	H	-3.8979	2.0713	0.0000
C	1.8010	-0.8380	0.0000	C	-7.8132	0.9971	0.0000	H	-4.8385	-2.8384	0.0000
C	0.7467	0.0544	0.0000	C	-8.0810	-0.4012	0.0000	H	-6.3161	2.5307	0.0000
C	1.0191	1.4605	0.0000	C	-7.0597	-1.3011	0.0000	H	-8.6576	1.6941	0.0000
C	-0.0863	2.3855	0.0000	H	8.7615	-1.9909	0.0000	H	-9.1232	-0.7370	0.0000
C	-1.3622	1.9425	0.0000	H	9.2231	0.4395	0.0000	H	-7.2558	-2.3793	0.0000

Table 3.522: Table of thermodynamic data as a function of temperature for Anthra[2,1-*a*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.174	522.431	522.431	∞
100	126.090	377.090	871.210	-49.412	551.961	607.762	-317.456
200	247.196	499.578	654.825	-31.050	536.298	669.816	-174.934
250	317.538	562.240	630.013	-16.943	528.960	704.045	-147.099
298.15	386.054	624.043	624.043	0.000	522.431	738.375	-129.357
300	388.654	626.439	624.050	0.717	522.191	739.713	-128.793
350	457.011	691.536	629.035	21.875	516.179	776.456	-115.877
400	520.419	756.763	640.927	46.335	510.965	813.993	-106.294
450	577.901	821.438	657.398	73.818	506.459	852.147	-98.913
500	629.332	885.040	676.993	104.023	502.567	890.793	-93.059
600	715.723	1007.727	721.983	171.446	496.288	969.062	-84.363
700	784.211	1123.398	771.153	246.572	491.782	1048.244	-78.219
800	839.269	1231.838	822.035	327.842	488.845	1127.945	-73.646
900	884.232	1333.371	873.271	414.090	487.278	1207.923	-70.105
1000	921.441	1428.520	924.089	504.431	486.892	1288.026	-67.278
1100	952.556	1517.845	974.049	598.176	487.466	1368.129	-64.966
1200	978.794	1601.885	1022.902	694.780	488.838	1448.124	-63.034
1300	1001.074	1681.134	1070.516	793.803	490.802	1527.992	-61.394
1400	1020.109	1756.036	1116.832	894.887	493.210	1607.695	-59.983
1500	1036.463	1826.988	1161.831	997.736	495.967	1687.215	-58.753
1600	1050.589	1894.342	1205.526	1102.105	498.927	1766.534	-57.670
1700	1062.850	1958.410	1247.945	1207.791	502.007	1845.636	-56.708
1800	1073.544	2019.470	1289.124	1314.623	505.123	1924.628	-55.850
1900	1082.913	2077.770	1329.109	1422.456	508.238	2003.387	-55.076
2000	1091.158	2133.531	1367.947	1531.168	511.290	2082.013	-54.375
2100	1098.444	2186.948	1405.684	1640.656	514.194	2160.473	-53.738
2200	1104.908	2238.200	1442.369	1750.830	516.947	2238.803	-53.155
2300	1110.665	2287.445	1478.047	1861.614	519.542	2317.009	-52.620
2400	1115.811	2334.825	1512.766	1972.942	521.901	2395.054	-52.126
2500	1120.427	2380.470	1546.567	2084.758	524.037	2473.130	-51.672
2600	1124.580	2424.496	1579.491	2197.012	525.909	2550.997	-51.249
2700	1128.330	2467.010	1611.580	2309.661	527.522	2628.876	-50.858
2800	1131.724	2508.107	1642.869	2422.666	528.847	2706.727	-50.494
2900	1134.806	2547.875	1673.394	2535.995	529.849	2784.475	-50.153
3000	1137.613	2586.395	1703.189	2649.618	530.580	2862.222	-49.835
3100	1140.174	2623.739	1732.284	2763.510	530.951	2939.867	-49.535
3200	1142.518	2659.976	1760.711	2877.646	531.009	3017.586	-49.256
3300	1144.668	2695.166	1788.498	2992.007	530.734	3095.351	-48.994
3400	1146.644	2729.368	1815.670	3106.574	530.095	3173.034	-48.747
3500	1148.464	2762.633	1842.253	3221.330	529.097	3250.722	-48.513
3600	1150.144	2795.010	1868.271	3336.262	527.763	3328.538	-48.295
3700	1151.698	2826.544	1893.746	3451.355	526.060	3406.417	-48.089
3800	1153.138	2857.277	1918.699	3566.598	523.958	3484.278	-47.894
3900	1154.474	2887.248	1943.151	3681.979	521.502	3562.145	-47.709
4000	1155.717	2916.493	1967.120	3797.489	518.675	3640.232	-47.536
4100	1156.874	2945.045	1990.625	3913.120	515.436	3718.312	-47.371
4200	1157.954	2972.936	2013.683	4028.862	511.817	3796.466	-47.215
4300	1158.962	3000.195	2036.309	4144.708	507.801	3874.611	-47.066
4400	1159.905	3026.850	2058.520	4260.652	503.400	3952.957	-46.927
4500	1160.789	3052.926	2080.329	4376.687	498.628	4031.469	-46.795
4600	1161.618	3078.448	2101.751	4492.808	493.429	4110.100	-46.671
4700	1162.397	3103.439	2122.798	4609.009	487.818	4188.722	-46.551
4800	1163.129	3127.919	2143.484	4725.286	481.848	4267.585	-46.440
4900	1163.819	3151.909	2163.820	4841.633	475.436	4346.426	-46.333
5000	1164.469	3175.428	2183.818	4958.048	468.685	4425.611	-46.233

3.523. Benzo[*b*]naphtho[1,2-*k*]chrysene



Other names: 4,5-Benz-10,11-(1',2'-naphtha)chrysene

Formula: C₃₀H₁₈

Mass: 378.464 g/mol

CAS Number: 214-15-3

Point Group: C_s

Length: 20.31 Å

Width: 8.728 Å

Breadth: 3.884 Å

L/B Ratio: 2.327

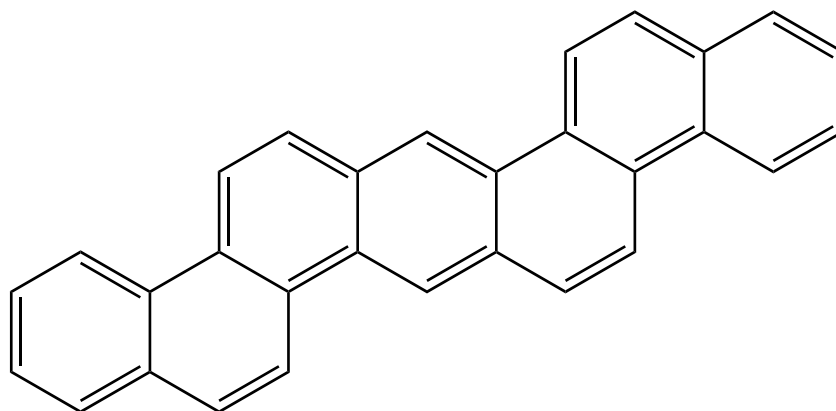
Cartesian coordinates:

C	7.5559	-1.5502	0.0000	C	-1.2589	-0.9279	0.0000	H	7.4097	1.8682	0.0000
C	7.9903	-0.1953	0.0000	C	-0.8203	0.4178	0.0000	H	5.8841	-2.8917	0.0000
C	7.0846	0.8217	0.0000	C	-1.7770	1.4437	0.0000	H	5.0658	2.6162	0.0000
C	6.2277	-1.8512	0.0000	C	-2.6311	-1.2144	0.0000	H	3.5377	-2.1435	0.0000
C	5.2489	-0.8081	0.0000	C	-3.5752	-0.1936	0.0000	H	2.7488	3.3705	0.0000
C	5.6818	0.5419	0.0000	C	-3.1375	1.1571	0.0000	H	0.3160	2.8550	0.0000
C	4.7309	1.5715	0.0000	C	-4.1137	2.2195	0.0000	H	-0.6476	-3.0198	0.0000
C	3.8774	-1.0953	0.0000	C	-5.4366	1.9495	0.0000	H	1.7875	-2.5084	0.0000
C	2.9309	-0.0742	0.0000	C	-4.9997	-0.4752	0.0000	H	-1.4320	2.4903	0.0000
C	3.3700	1.2791	0.0000	C	-5.9164	0.5899	0.0000	H	-2.9771	-2.2608	0.0000
C	2.3927	2.3338	0.0000	C	-7.2980	0.3192	0.0000	H	-3.7478	3.2528	0.0000
C	1.0693	2.0522	0.0000	C	-7.7521	-0.9835	0.0000	H	-6.1786	2.7564	0.0000
C	1.5088	-0.3516	0.0000	C	-6.8399	-2.0473	0.0000	H	-8.0084	1.1538	0.0000
C	0.5960	0.6962	0.0000	C	-5.4837	-1.7972	0.0000	H	-8.8268	-1.1926	0.0000
C	-0.2907	-1.9836	0.0000	H	8.3095	-2.3445	0.0000	H	-7.2095	-3.0779	0.0000
C	1.0367	-1.7032	0.0000	H	9.0653	0.0128	0.0000	H	-4.7545	-2.6220	0.0000

Table 3.523: Table of thermodynamic data as a function of temperature for Benzo[*b*]naphtho[1,2-*k*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.670	490.854	490.854	∞
100	127.785	385.178	881.918	-49.674	520.122	575.115	-300.403
200	248.418	508.629	664.505	-31.175	504.595	636.303	-166.182
250	318.811	571.567	639.596	-17.007	497.319	670.072	-140.001
298.15	387.439	633.603	633.603	0.000	490.854	703.947	-123.326
300	390.044	636.008	633.611	0.719	490.616	705.268	-122.795
350	458.516	701.328	638.613	21.950	484.677	741.526	-110.664
400	521.998	766.762	650.545	46.487	479.540	778.569	-101.669
450	579.503	831.625	667.069	74.050	475.114	816.218	-94.742
500	630.913	895.395	686.724	104.335	471.302	854.351	-89.252
600	717.176	1018.360	731.842	171.911	465.176	931.570	-81.099
700	785.486	1134.242	781.138	247.173	460.806	1009.677	-75.342
800	840.364	1242.840	832.138	328.561	457.988	1088.285	-71.056
900	885.163	1344.493	883.481	414.911	456.521	1167.157	-67.739
1000	922.233	1439.732	934.395	505.337	456.221	1246.143	-65.090
1100	953.231	1529.127	984.441	599.155	456.869	1325.121	-62.923
1200	979.373	1613.222	1033.370	695.822	458.303	1403.985	-61.113
1300	1001.573	1692.514	1081.053	794.899	460.321	1482.717	-59.575
1400	1020.542	1767.450	1127.430	896.029	462.775	1561.280	-58.251
1500	1036.842	1838.430	1172.485	998.918	465.573	1639.658	-57.097
1600	1050.922	1905.807	1216.230	1103.323	468.569	1717.831	-56.080
1700	1063.145	1969.894	1258.693	1209.041	471.680	1795.786	-55.177
1800	1073.807	2030.970	1299.914	1315.901	474.824	1873.628	-54.370
1900	1083.149	2089.284	1339.937	1423.758	477.964	1951.237	-53.642
2000	1091.371	2145.056	1378.809	1532.493	481.038	2028.711	-52.983
2100	1098.636	2198.483	1416.578	1642.001	483.962	2106.018	-52.383
2200	1105.083	2249.743	1453.292	1752.193	486.733	2183.194	-51.835
2300	1110.825	2298.995	1488.998	1862.994	489.345	2260.245	-51.331
2400	1115.957	2346.382	1523.741	1974.338	491.720	2337.135	-50.865
2500	1120.561	2392.033	1557.566	2086.168	493.870	2414.056	-50.438
2600	1124.704	2436.064	1590.512	2198.435	495.755	2490.766	-50.039
2700	1128.444	2478.582	1622.621	2311.095	497.379	2567.488	-49.670
2800	1131.830	2519.683	1653.929	2424.112	498.715	2644.181	-49.327
2900	1134.905	2559.455	1684.472	2537.451	499.728	2720.771	-49.005
3000	1137.705	2597.978	1714.284	2651.083	500.468	2797.361	-48.705
3100	1140.260	2635.325	1743.395	2764.984	500.848	2873.847	-48.423
3200	1142.599	2671.565	1771.837	2879.128	500.914	2950.407	-48.159
3300	1144.743	2706.758	1799.637	2993.497	500.647	3027.013	-47.913
3400	1146.715	2740.961	1826.823	3108.071	500.015	3103.537	-47.679
3500	1148.531	2774.228	1853.418	3222.835	499.024	3180.065	-47.459
3600	1150.208	2806.607	1879.448	3337.773	497.697	3256.722	-47.253
3700	1151.758	2838.143	1904.935	3452.872	496.000	3333.441	-47.059
3800	1153.195	2868.878	1929.899	3568.121	493.904	3410.142	-46.875
3900	1154.528	2898.850	1954.361	3683.507	491.454	3486.848	-46.700
4000	1155.768	2928.096	1978.340	3799.023	488.631	3563.775	-46.537
4100	1156.923	2956.649	2001.855	3914.658	485.397	3640.695	-46.382
4200	1158.000	2984.541	2024.921	4030.405	481.783	3717.688	-46.235
4300	1159.006	3011.802	2047.556	4146.256	477.772	3794.673	-46.095
4400	1159.947	3038.458	2069.775	4262.204	473.375	3871.858	-45.964
4500	1160.829	3064.535	2091.592	4378.243	468.608	3949.210	-45.840
4600	1161.657	3090.058	2113.021	4494.368	463.412	4026.679	-45.723
4700	1162.434	3115.049	2134.076	4610.573	457.805	4104.140	-45.611
4800	1163.164	3139.530	2154.769	4726.853	451.839	4181.842	-45.507
4900	1163.852	3163.521	2175.112	4843.205	445.430	4259.522	-45.406
5000	1164.501	3187.040	2195.116	4959.623	438.683	4337.546	-45.313

3.524. Phenanthro[1,2-*b*]chrysene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 220-78-0
Point Group: C_{2h}

Length: 20.30 Å
Width: 8.728 Å
Breadth: 3.883 Å
L/B Ratio: 2.326

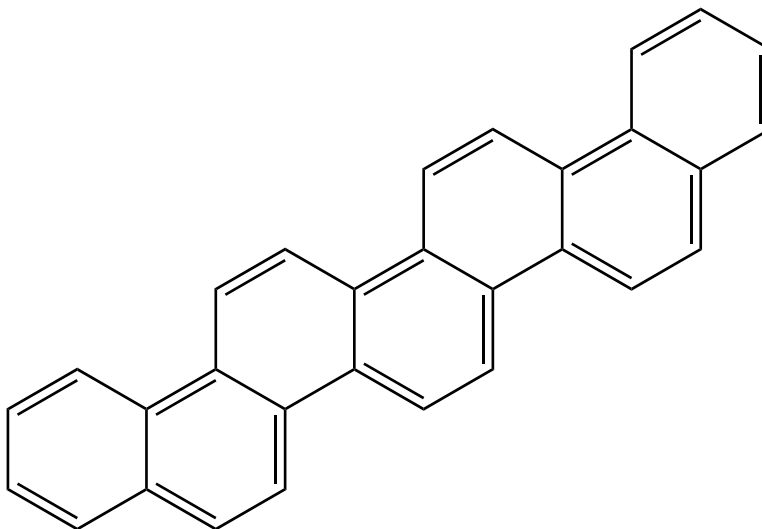
Cartesian coordinates:

C	7.3945	-1.1842	0.0000	C	-1.3883	-0.2590	0.0000	H	7.3616	2.2270	0.0000
C	7.8756	0.1407	0.0000	C	-0.9029	1.0732	0.0000	H	5.6578	-2.4609	0.0000
C	6.9963	1.1937	0.0000	C	-1.8385	2.1634	0.0000	H	5.0715	3.0718	0.0000
C	6.0453	-1.4307	0.0000	C	-3.1721	1.9305	0.0000	H	2.6168	2.6521	0.0000
C	5.1143	-0.3622	0.0000	C	-2.8173	-0.4892	0.0000	H	1.4445	-3.1862	0.0000
C	5.5991	0.9595	0.0000	C	-3.6945	0.5931	0.0000	H	3.8960	-2.7600	0.0000
C	4.6768	2.0494	0.0000	C	-4.6767	-2.0495	0.0000	H	0.8510	2.3484	0.0000
C	3.3366	1.8191	0.0000	C	-3.3365	-1.8191	0.0000	H	-0.8510	-2.3483	0.0000
C	3.6946	-0.5932	0.0000	C	-5.5991	-0.9596	0.0000	H	-1.4446	3.1862	0.0000
C	2.8174	0.4892	0.0000	C	-5.1143	0.3621	0.0000	H	-3.8961	2.7599	0.0000
C	1.8385	-2.1634	0.0000	C	-6.0452	1.4307	0.0000	H	-5.0714	-3.0719	0.0000
C	3.1721	-1.9305	0.0000	C	-7.3946	1.1843	0.0000	H	-2.6166	-2.6521	0.0000
C	0.9029	-1.0732	0.0000	C	-7.8757	-0.1407	0.0000	H	-5.6577	2.4609	0.0000
C	1.3883	0.2590	0.0000	C	-6.9963	-1.1938	0.0000	H	-8.1089	2.0140	0.0000
C	0.4723	1.3135	0.0000	H	8.1089	-2.0140	0.0000	H	-8.9559	-0.3190	0.0000
C	-0.4724	-1.3134	0.0000	H	8.9559	0.3190	0.0000	H	-7.3616	-2.2270	0.0000

Table 3.524: Table of thermodynamic data as a function of temperature for Phenanthro[1,2-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	Δ _f <i>H</i> ^o	Δ _f <i>G</i> ^o	log <i>K</i> _f
0	0.0	0.0	∞	-57.869	483.633	483.633	∞
100	128.743	384.908	882.297	-49.739	512.836	567.855	-296.611
200	248.714	508.798	664.701	-31.181	497.368	629.042	-164.286
250	318.852	571.774	639.791	-17.004	490.100	662.802	-138.482
298.15	387.288	633.800	633.800	0.000	483.633	696.667	-122.051
300	389.886	636.204	633.807	0.719	483.395	697.987	-121.528
350	458.229	701.489	638.807	21.939	477.443	734.237	-109.577
400	521.638	766.879	650.732	46.459	472.291	771.273	-100.716
450	579.108	831.697	667.246	74.003	467.846	808.917	-93.895
500	630.505	895.425	686.889	104.268	464.013	847.047	-88.489
600	716.771	1018.315	731.978	171.802	457.846	924.267	-80.463
700	785.093	1134.136	781.243	247.025	453.436	1002.382	-74.797
800	839.984	1242.682	832.214	328.375	450.579	1081.003	-70.581
900	884.796	1344.291	883.528	414.687	449.075	1159.893	-67.317
1000	921.879	1439.493	934.416	505.077	448.740	1238.901	-64.712
1100	952.893	1528.854	984.436	598.861	449.352	1317.905	-62.581
1200	979.051	1612.920	1033.342	695.494	450.754	1396.798	-60.800
1300	1001.268	1692.187	1081.003	794.540	452.740	1475.561	-59.288
1400	1020.255	1767.102	1127.359	895.640	455.165	1554.158	-57.985
1500	1036.573	1838.063	1172.395	998.502	457.935	1632.572	-56.850
1600	1050.670	1905.422	1216.122	1102.881	460.905	1710.782	-55.850
1700	1062.909	1969.495	1258.569	1208.574	463.992	1788.777	-54.961
1800	1073.586	2030.558	1299.774	1315.411	467.112	1866.659	-54.168
1900	1082.942	2088.860	1339.782	1423.247	470.231	1944.310	-53.452
2000	1091.177	2144.621	1378.640	1531.962	473.285	2021.827	-52.804
2100	1098.455	2198.040	1416.397	1641.451	476.190	2099.178	-52.213
2200	1104.913	2249.292	1453.098	1751.625	478.944	2176.398	-51.673
2300	1110.666	2298.537	1488.793	1862.410	481.540	2253.495	-51.177
2400	1115.808	2345.917	1523.526	1973.738	483.899	2330.431	-50.719
2500	1120.421	2391.561	1557.340	2085.554	486.034	2407.399	-50.299
2600	1124.572	2435.587	1590.277	2197.807	487.906	2484.156	-49.906
2700	1128.320	2478.101	1622.377	2310.455	489.517	2560.926	-49.543
2800	1131.713	2519.197	1653.676	2423.459	490.841	2637.667	-49.205
2900	1134.795	2558.965	1684.211	2536.787	491.843	2714.307	-48.889
3000	1137.600	2597.484	1714.015	2650.409	492.572	2790.945	-48.594
3100	1140.161	2634.829	1743.119	2764.299	492.942	2867.481	-48.316
3200	1142.505	2671.065	1771.554	2878.434	492.999	2944.091	-48.056
3300	1144.654	2706.255	1799.348	2992.793	492.722	3020.747	-47.813
3400	1146.630	2740.456	1826.527	3107.359	492.082	3097.322	-47.584
3500	1148.451	2773.721	1853.116	3222.114	491.082	3173.900	-47.367
3600	1150.131	2806.097	1879.140	3337.044	489.747	3250.608	-47.164
3700	1151.685	2837.631	1904.621	3452.136	488.043	3327.378	-46.973
3800	1153.125	2868.364	1929.580	3567.378	485.939	3404.131	-46.792
3900	1154.462	2898.334	1954.038	3682.758	483.483	3480.888	-46.620
4000	1155.705	2927.579	1978.012	3798.267	480.654	3557.867	-46.460
4100	1156.862	2956.130	2001.522	3913.896	477.414	3634.838	-46.307
4200	1157.942	2984.021	2024.584	4029.637	473.793	3711.884	-46.163
4300	1158.951	3011.280	2047.214	4145.482	469.777	3788.921	-46.025
4400	1159.894	3037.935	2069.429	4261.425	465.374	3866.158	-45.896
4500	1160.778	3064.011	2091.242	4377.459	460.601	3943.562	-45.775
4600	1161.608	3089.533	2112.668	4493.578	455.401	4021.084	-45.660
4700	1162.387	3114.523	2133.719	4609.779	449.789	4098.598	-45.550
4800	1163.119	3139.003	2154.408	4726.054	443.818	4176.352	-45.447
4900	1163.809	3162.993	2174.748	4842.401	437.405	4254.085	-45.348
5000	1164.459	3186.511	2194.748	4958.815	430.653	4332.162	-45.257

3.525. Dibenzo[*c,m*]picene



Formula: C₃₀H₁₈
Mass: 378.464 g/mol
CAS Number: 13109-47-2
Point Group: C_{2v}

Length: 20.17 Å
Width: 7.967 Å
Breadth: 3.883 Å
L/B Ratio: 2.532

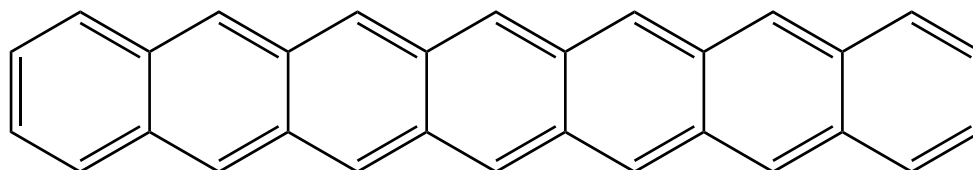
Cartesian coordinates:

C	7.1030	-1.6736	0.0000	C	-0.7196	-0.4913	0.0000	H	7.6252	1.6967	0.0000
C	7.7925	-0.4467	0.0000	C	-1.4173	0.7238	0.0000	H	5.1783	-2.6488	0.0000
C	7.0955	0.7373	0.0000	C	-2.8145	-1.7125	0.0000	H	5.5039	2.9043	0.0000
C	5.7296	-1.6961	0.0000	C	-1.4526	-1.7127	0.0000	H	3.0184	2.8955	0.0000
C	4.9885	-0.4911	0.0000	C	-3.5458	-0.4911	0.0000	H	0.8904	-2.6573	0.0000
C	5.6812	0.7329	0.0000	C	-2.8527	0.7236	0.0000	H	3.3846	-2.6532	0.0000
C	4.9457	1.9611	0.0000	C	-3.5902	1.9518	0.0000	H	1.2429	2.8927	0.0000
C	3.5889	1.9542	0.0000	C	-4.9470	1.9577	0.0000	H	-1.2448	2.8919	0.0000
C	3.5461	-0.4887	0.0000	C	-4.9882	-0.4945	0.0000	H	-3.3827	-2.6555	0.0000
C	2.8523	0.7255	0.0000	C	-5.6817	0.7291	0.0000	H	-0.8886	-2.6579	0.0000
C	1.4537	-1.7117	0.0000	C	-7.0960	0.7326	0.0000	H	-3.0203	2.8935	0.0000
C	2.8157	-1.7106	0.0000	C	-7.7923	-0.4519	0.0000	H	-5.5058	2.9006	0.0000
C	0.7200	-0.4908	0.0000	C	-7.1019	-1.6784	0.0000	H	-7.6263	1.6916	0.0000
C	1.4168	0.7248	0.0000	C	-5.7285	-1.7000	0.0000	H	-8.8871	-0.4515	0.0000
C	0.6788	1.9476	0.0000	H	7.6712	-2.6095	0.0000	H	-7.6696	-2.6146	0.0000
C	-0.6800	1.9471	0.0000	H	8.8874	-0.4457	0.0000	H	-5.1766	-2.6523	0.0000

Table 3.525: Table of thermodynamic data as a function of temperature for Dibenzo[*c,m*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K</i> _{<i>f</i>}
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-57.412	479.690	479.690	∞
100	127.782	373.816	868.655	-49.484	509.148	565.277	-295.264
200	247.373	496.927	652.129	-31.040	493.566	627.614	-163.913
250	317.405	559.591	627.327	-16.934	486.228	661.975	-138.309
298.15	385.830	621.360	621.360	0.000	479.690	696.433	-122.010
300	388.430	623.755	621.367	0.716	479.449	697.777	-121.491
350	456.831	688.819	626.350	21.864	473.427	734.655	-109.639
400	520.334	754.029	638.236	46.317	468.206	772.328	-100.854
450	577.910	818.699	654.703	73.799	463.699	810.619	-94.092
500	629.411	882.306	674.293	104.006	459.809	849.402	-88.735
600	715.855	1005.014	719.279	171.441	453.542	927.943	-80.783
700	784.312	1120.703	768.449	246.578	449.048	1007.396	-75.171
800	839.302	1229.152	819.333	327.855	446.118	1087.365	-70.996
900	884.191	1330.686	870.571	414.103	444.549	1167.612	-67.765
1000	921.335	1425.827	921.390	504.436	444.156	1247.984	-65.187
1100	952.400	1515.139	971.350	598.168	444.717	1328.357	-63.077
1200	978.602	1599.164	1020.202	694.754	446.072	1408.623	-61.315
1300	1000.859	1678.396	1067.814	793.757	448.015	1488.764	-59.818
1400	1019.880	1753.282	1114.126	894.819	450.401	1568.742	-58.529
1500	1036.228	1824.218	1159.122	997.644	453.134	1648.538	-57.406
1600	1050.353	1891.556	1202.813	1101.990	456.071	1728.135	-56.417
1700	1062.617	1955.610	1245.226	1207.653	459.128	1807.517	-55.537
1800	1073.316	2016.657	1286.401	1314.462	462.221	1886.788	-54.752
1900	1082.693	2074.945	1326.381	1422.272	465.313	1965.830	-54.043
2000	1090.946	2130.695	1365.213	1530.963	468.344	2044.739	-53.402
2100	1098.241	2184.102	1402.945	1640.429	471.227	2123.483	-52.818
2200	1104.714	2235.345	1439.625	1750.583	473.960	2202.098	-52.283
2300	1110.480	2284.581	1475.299	1861.349	476.536	2280.590	-51.793
2400	1115.634	2331.953	1510.012	1972.659	478.877	2358.921	-51.340
2500	1120.258	2377.591	1543.808	2084.458	480.996	2437.286	-50.923
2600	1124.420	2421.611	1576.728	2196.695	482.851	2515.441	-50.535
2700	1128.177	2464.118	1608.812	2309.328	484.448	2593.609	-50.175
2800	1131.579	2505.210	1640.096	2422.319	485.758	2671.748	-49.841
2900	1134.668	2544.973	1670.617	2535.634	486.747	2749.787	-49.528
3000	1137.481	2583.489	1700.408	2649.243	487.463	2827.825	-49.236
3100	1140.049	2620.829	1729.499	2763.122	487.822	2905.760	-48.961
3200	1142.399	2657.062	1757.922	2877.246	487.868	2983.770	-48.704
3300	1144.554	2692.249	1785.705	2991.595	487.581	3061.827	-48.464
3400	1146.535	2726.447	1812.873	3106.151	486.931	3139.802	-48.236
3500	1148.360	2759.709	1839.452	3220.897	485.922	3217.782	-48.022
3600	1150.045	2792.083	1865.467	3335.818	484.578	3295.891	-47.821
3700	1151.603	2823.614	1890.938	3450.902	482.866	3374.062	-47.632
3800	1153.047	2854.345	1915.889	3566.135	480.754	3452.217	-47.453
3900	1154.387	2884.314	1940.337	3681.507	478.290	3530.376	-47.283
4000	1155.634	2913.556	1964.304	3797.009	475.453	3608.757	-47.125
4100	1156.794	2942.106	1987.806	3912.631	472.207	3687.131	-46.974
4200	1157.877	2969.995	2010.861	4028.366	468.580	3765.579	-46.831
4300	1158.889	2997.253	2033.484	4144.204	464.557	3844.018	-46.695
4400	1159.835	3023.906	2055.692	4260.141	460.148	3922.658	-46.567
4500	1160.721	3049.981	2077.499	4376.169	455.370	4001.465	-46.447
4600	1161.553	3075.501	2098.918	4492.284	450.164	4080.390	-46.333
4700	1162.334	3100.490	2119.963	4608.478	444.547	4159.307	-46.225
4800	1163.069	3124.969	2140.647	4724.749	438.570	4238.465	-46.123
4900	1163.760	3148.958	2160.980	4841.091	432.152	4317.602	-46.025
5000	1164.412	3172.476	2180.976	4957.500	425.396	4397.082	-45.935

3.526. Heptacene



Formula: $C_{30}H_{18}$
Mass: 378.464 g/mol
CAS Number: 258-38-8
Point Group: D_{2h}

Length: 21.38 Å
Width: 7.434 Å
Breadth: 3.882 Å
L/B Ratio: 2.876

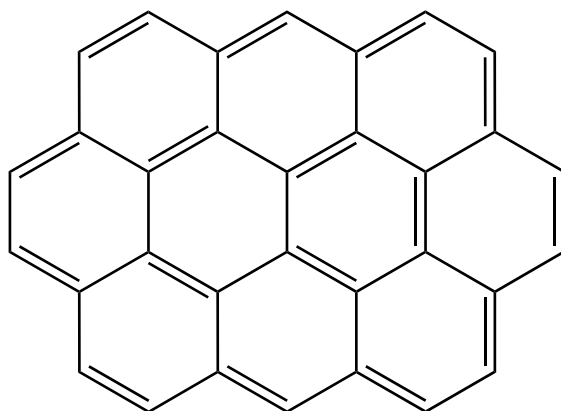
Cartesian coordinates:

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C	-7.3620	-1.4084	0.0000	C	2.4527	-1.4071	0.0000	H	-4.8979	-2.5057	0.0000
C	-7.3617	1.4102	0.0000	C	2.4530	1.4064	0.0000	H	-4.8972	2.5069	0.0000
C	-6.0902	0.7222	0.0000	C	3.6531	0.7177	0.0000	H	-2.4485	-2.5037	0.0000
C	-6.0904	-0.7207	0.0000	C	3.6529	-0.7186	0.0000	H	-2.4479	2.5042	0.0000
C	-4.9056	-1.4087	0.0000	C	4.9052	-1.4098	0.0000	H	-0.0003	-2.5030	0.0000
C	-4.9053	1.4098	0.0000	C	4.9055	1.4086	0.0000	H	0.0003	2.5030	0.0000
C	-3.6528	0.7186	0.0000	C	6.0904	0.7206	0.0000	H	2.4479	-2.5042	0.0000
C	-3.6530	-0.7178	0.0000	C	6.0903	-0.7221	0.0000	H	2.4485	2.5036	0.0000
C	-2.4532	-1.4065	0.0000	C	7.3616	-1.4101	0.0000	H	4.8972	-2.5069	0.0000
C	-2.4528	1.4071	0.0000	C	8.5234	-0.7194	0.0000	H	4.8978	2.5057	0.0000
C	-1.2171	0.7159	0.0000	C	8.5236	0.7174	0.0000	H	7.3516	-2.5061	0.0000
C	-1.2172	-0.7156	0.0000	C	7.3620	1.4084	0.0000	H	9.4882	-1.2370	0.0000
C	-0.0002	-1.4058	0.0000	H	-9.4882	1.2371	0.0000	H	9.4885	1.2348	0.0000
C	0.0001	1.4058	0.0000	H	-9.4885	-1.2347	0.0000	H	7.3522	2.5043	0.0000

Table 3.526: Table of thermodynamic data as a function of temperature for Heptacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-57.187	596.905	596.905	∞
100	125.030	361.846	857.504	-49.566	626.281	683.607	-357.072
200	248.106	484.187	640.253	-31.213	610.608	747.204	-195.146
250	319.271	547.147	615.305	-17.040	603.338	782.196	-163.428
298.15	388.269	609.300	609.300	0.000	596.905	817.244	-143.175
300	390.882	611.710	609.308	0.721	596.669	818.610	-142.530
350	459.459	677.170	614.321	21.997	590.775	856.080	-127.760
400	522.910	742.728	626.277	46.581	585.685	894.327	-116.785
450	580.335	807.695	642.834	74.187	581.303	933.175	-108.318
500	631.661	871.548	662.523	104.512	577.529	972.502	-101.595
600	717.795	994.637	707.712	172.155	571.471	1052.099	-91.591
700	786.040	1110.609	757.072	247.476	567.160	1132.575	-84.512
800	840.890	1219.278	808.131	328.918	564.395	1213.542	-79.235
900	885.678	1320.993	859.527	415.319	562.981	1294.767	-75.145
1000	922.738	1416.286	910.489	505.797	562.732	1376.100	-71.879
1100	953.725	1505.728	960.578	599.665	563.429	1457.421	-69.206
1200	979.852	1589.865	1009.548	696.380	564.912	1538.622	-66.973
1300	1002.034	1669.195	1057.269	795.504	566.977	1619.688	-65.079
1400	1020.983	1744.165	1103.680	896.679	569.477	1700.581	-63.448
1500	1037.261	1815.175	1148.767	999.612	572.317	1781.286	-62.029
1600	1051.319	1882.578	1192.542	1104.058	575.354	1861.783	-60.780
1700	1063.519	1946.688	1235.033	1209.814	578.504	1942.060	-59.671
1800	1074.159	2007.785	1276.280	1316.709	581.684	2022.222	-58.682
1900	1083.480	2066.117	1316.327	1424.602	584.858	2102.148	-57.791
2000	1091.682	2121.905	1355.221	1533.368	587.965	2181.938	-56.985
2100	1098.929	2175.348	1393.011	1642.906	590.918	2261.560	-56.252
2200	1105.359	2226.621	1429.745	1753.127	593.718	2341.048	-55.582
2300	1111.084	2275.885	1465.470	1863.954	596.357	2420.411	-54.968
2400	1116.201	2323.282	1500.231	1975.323	598.757	2499.611	-54.401
2500	1120.791	2368.943	1534.072	2087.177	600.930	2578.841	-53.881
2600	1124.921	2412.983	1567.034	2199.466	602.838	2657.860	-53.396
2700	1128.649	2455.509	1599.158	2312.148	604.483	2736.890	-52.947
2800	1132.024	2496.617	1630.480	2425.184	605.839	2815.890	-52.530
2900	1135.088	2536.396	1661.036	2538.542	606.871	2894.786	-52.140
3000	1137.878	2574.925	1690.860	2652.193	607.628	2973.681	-51.775
3100	1140.424	2612.277	1719.984	2766.110	608.025	3052.473	-51.433
3200	1142.754	2648.522	1748.437	2880.270	608.108	3131.337	-51.113
3300	1144.891	2683.719	1776.248	2994.654	607.855	3210.247	-50.813
3400	1146.855	2717.927	1803.444	3109.243	607.238	3289.075	-50.529
3500	1148.665	2751.198	1830.050	3224.020	606.260	3367.906	-50.262
3600	1150.335	2783.581	1856.089	3338.971	604.946	3446.866	-50.012
3700	1151.879	2815.120	1881.584	3454.083	603.262	3525.887	-49.776
3800	1153.310	2845.858	1906.557	3569.343	601.177	3604.891	-49.552
3900	1154.639	2875.833	1931.028	3684.741	598.739	3683.899	-49.339
4000	1155.874	2905.082	1955.015	3800.268	595.927	3763.127	-49.140
4100	1157.024	2933.638	1978.537	3915.913	592.704	3842.348	-48.951
4200	1158.097	2961.532	2001.611	4031.670	589.099	3921.643	-48.772
4300	1159.099	2988.795	2024.253	4147.530	585.098	4000.928	-48.601
4400	1160.036	3015.453	2046.478	4263.488	580.710	4080.414	-48.440
4500	1160.915	3041.532	2068.302	4379.536	575.951	4160.066	-48.288
4600	1161.739	3067.057	2089.737	4495.669	570.764	4239.835	-48.144
4700	1162.513	3092.050	2110.798	4611.882	565.165	4319.597	-48.006
4800	1163.240	3116.532	2131.497	4728.170	559.206	4399.598	-47.876
4900	1163.925	3140.525	2151.845	4844.528	552.805	4479.578	-47.752
5000	1164.571	3164.046	2171.855	4960.953	546.065	4559.902	-47.636

3.527. Ovalene



Formula: C₃₂H₁₄
Mass: 398.454 g/mol
CAS Number: 190-26-1
Point Group: D_{2h}

Length: 14.07 Å
Width: 11.66 Å
Breadth: 3.885 Å
L/B Ratio: 1.207

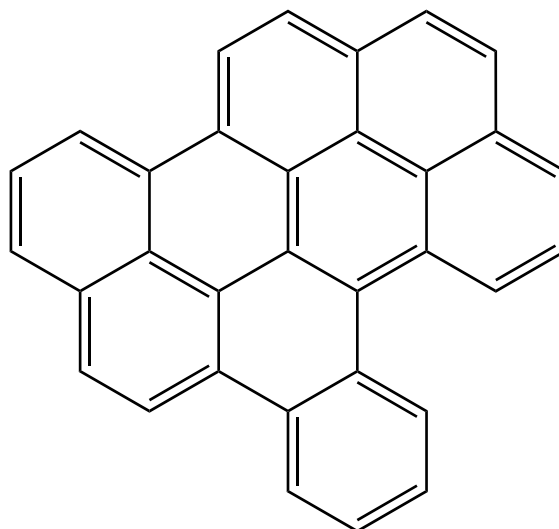
Cartesian coordinates:

C	-3.6537	-2.8442	0.0000	C	1.2193	1.4243	0.0000	H	-4.6129	-3.3747	0.0000
C	-2.4821	-3.5271	0.0000	C	1.2179	2.8399	0.0000	H	-2.4715	-4.6232	0.0000
C	-1.2179	-2.8399	0.0000	C	0.0034	3.5325	0.0000	H	-0.0044	-4.6295	0.0000
C	-0.0034	-3.5325	0.0000	C	0.0007	0.7197	0.0000	H	2.4626	-4.6279	0.0000
C	1.2125	-2.8422	0.0000	C	-1.2166	1.4266	0.0000	H	4.6065	-3.3835	0.0000
C	2.4754	-3.5318	0.0000	C	-1.2125	2.8422	0.0000	H	-5.8350	1.2457	0.0000
C	3.6483	-2.8511	0.0000	C	-2.4754	3.5318	0.0000	H	-5.8373	-1.2346	0.0000
C	-3.6771	-1.4074	0.0000	C	-3.6483	2.8511	0.0000	H	4.6129	3.3747	0.0000
C	-4.8888	0.6925	0.0000	C	-3.6744	1.4144	0.0000	H	2.4714	4.6232	0.0000
C	-4.8901	-0.6831	0.0000	C	-2.4593	0.7127	0.0000	H	0.0044	4.6294	0.0000
C	-2.4606	-0.7080	0.0000	C	2.4606	0.7080	0.0000	H	-2.4626	4.6279	0.0000
C	-1.2194	-1.4243	0.0000	C	2.4593	-0.7127	0.0000	H	-4.6064	3.3835	0.0000
C	-0.0007	-0.7197	0.0000	C	3.6745	-1.4144	0.0000	H	5.8350	-1.2457	0.0000
C	1.2166	-1.4266	0.0000	C	4.8888	-0.6924	0.0000	H	5.8373	1.2346	0.0000
C	3.6537	2.8442	0.0000	C	4.8901	0.6832	0.0000				
C	2.4821	3.5271	0.0000	C	3.6771	1.4074	0.0000				

Table 3.527: Table of thermodynamic data as a function of temperature for Ovalene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-51.508	414.465	414.465	∞
100	101.695	326.981	782.171	-45.519	438.934	479.792	-250.612
200	228.450	434.383	580.874	-29.298	425.865	525.890	-137.346
250	299.851	493.000	557.390	-16.098	419.822	551.594	-115.247
298.15	368.518	551.708	551.708	0.000	414.465	577.474	-101.169
300	371.115	553.995	551.715	0.684	414.267	578.483	-100.721
350	439.263	616.375	556.486	20.961	409.329	606.254	-90.477
400	502.383	679.214	567.899	44.526	405.031	634.676	-82.878
450	559.576	741.748	583.747	71.101	401.282	663.612	-77.028
500	610.713	803.404	602.639	100.383	397.994	692.963	-72.392
600	696.356	922.635	646.121	165.908	392.521	752.497	-65.509
700	763.743	1035.243	693.749	239.045	388.356	812.847	-60.654
800	817.343	1140.858	743.109	318.199	385.366	873.694	-57.045
900	860.595	1239.712	792.856	402.170	383.400	934.845	-54.256
1000	895.969	1332.276	842.220	490.056	382.321	996.181	-52.034
1100	925.231	1419.086	890.758	581.161	381.945	1057.603	-50.220
1200	949.672	1500.671	938.219	674.942	382.148	1119.010	-48.708
1300	970.254	1577.521	984.469	770.967	382.758	1180.396	-47.428
1400	987.715	1650.081	1029.446	868.889	383.652	1241.727	-46.328
1500	1002.626	1718.748	1073.131	968.425	384.764	1302.990	-45.373
1600	1015.439	1783.875	1115.535	1069.344	385.966	1364.163	-44.534
1700	1026.512	1845.776	1156.685	1171.455	387.195	1425.236	-43.791
1800	1036.133	1904.728	1196.618	1274.598	388.376	1486.308	-43.131
1900	1044.535	1960.979	1235.379	1378.641	389.487	1547.256	-42.536
2000	1051.908	2014.748	1273.013	1483.471	390.479	1608.179	-42.000
2100	1058.407	2066.232	1309.568	1588.993	391.272	1669.041	-41.514
2200	1064.161	2115.604	1345.092	1695.127	391.869	1729.869	-41.071
2300	1069.276	2163.023	1379.630	1801.804	392.273	1790.679	-40.667
2400	1073.840	2208.629	1413.228	1908.964	392.406	1851.418	-40.294
2500	1077.928	2252.550	1445.927	2016.556	392.288	1912.285	-39.954
2600	1081.601	2294.900	1477.771	2124.536	391.881	1973.030	-39.638
2700	1084.913	2335.783	1508.796	2232.865	391.194	2033.885	-39.347
2800	1087.909	2375.294	1539.041	2341.508	390.199	2094.786	-39.078
2900	1090.627	2413.518	1568.540	2450.437	388.866	2155.673	-38.827
3000	1093.099	2450.534	1597.326	2559.625	387.247	2216.643	-38.594
3100	1095.353	2486.414	1625.430	2669.050	385.255	2277.578	-38.376
3200	1097.415	2521.223	1652.883	2778.689	382.941	2338.671	-38.174
3300	1099.304	2555.022	1679.711	2888.527	380.286	2399.890	-37.986
3400	1101.040	2587.866	1705.940	2998.545	377.257	2461.088	-37.809
3500	1102.638	2619.805	1731.597	3108.730	373.863	2522.361	-37.643
3600	1104.113	2650.889	1756.703	3219.069	370.130	2583.844	-37.490
3700	1105.476	2681.159	1781.281	3329.549	366.022	2645.445	-37.346
3800	1106.738	2710.657	1805.352	3440.161	361.515	2707.103	-37.211
3900	1107.909	2739.420	1828.935	3550.894	356.651	2768.815	-37.083
4000	1108.998	2767.484	1852.049	3661.740	351.415	2830.823	-36.966
4100	1110.012	2794.881	1874.712	3772.691	345.767	2892.881	-36.855
4200	1110.957	2821.641	1896.941	3883.740	339.739	2955.071	-36.751
4300	1111.839	2847.793	1918.751	3994.880	333.317	3017.306	-36.652
4400	1112.665	2873.363	1940.157	4106.106	326.510	3079.797	-36.561
4500	1113.438	2898.376	1961.174	4217.411	319.337	3142.509	-36.477
4600	1114.163	2922.857	1981.815	4328.792	311.735	3205.404	-36.398
4700	1114.844	2946.825	2002.093	4440.242	303.726	3268.334	-36.323
4800	1115.484	2970.303	2022.020	4551.759	295.358	3331.562	-36.254
4900	1116.087	2993.310	2041.609	4663.338	286.548	3394.809	-36.188
5000	1116.655	3015.864	2060.869	4774.975	277.405	3458.450	-36.129

3.528. Dibenzo[*a,ghi*]naphtho[2,1,8-*cde*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 57789-81-8
Point Group: C₁

Length: 13.80 Å
Width: 12.80 Å
Breadth: 5.045 Å
L/B Ratio: 1.078

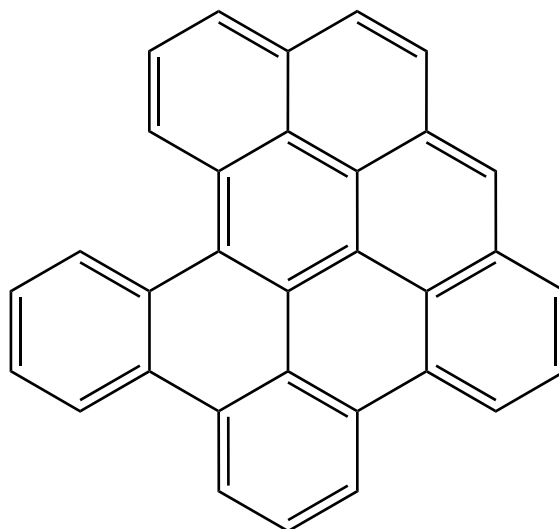
Cartesian coordinates:

C	-1.0726	-3.5637	-0.5284	C	-4.4382	-1.4481	0.7589	H	-5.1478	-2.2203	1.0749
C	-0.2358	-2.4801	-0.1568	C	-3.0883	-1.7691	0.6368	H	-5.9529	0.0730	0.5399
C	1.1464	-2.7396	-0.0397	C	-2.0928	2.8951	-0.3069	H	-2.7747	-2.7961	0.8688
C	1.6241	-4.0695	-0.1491	C	-3.5040	3.1659	-0.3278	H	-5.4759	2.3788	-0.0972
C	0.7766	-5.1044	-0.4482	C	-4.3988	2.1760	-0.1041	H	-3.8318	4.1952	-0.5128
C	-0.5862	-4.8387	-0.6710	C	0.6595	2.3511	-0.1516	H	-1.5063	4.9631	-0.5744
C	2.0689	-1.6519	0.1289	C	0.1917	3.6641	-0.3359	H	0.9282	4.4800	-0.4029
C	1.5952	-0.3415	0.0711	C	-1.1566	3.9352	-0.4256	H	5.4278	-1.0522	0.4896
C	0.1836	-0.0854	0.0117	C	2.5283	0.7476	0.0978	H	3.8105	-2.9343	0.3738
C	-0.7313	-1.1354	0.0287	C	3.9074	0.4878	0.2382	H	2.6674	4.1595	-0.1211
C	-0.2558	1.2899	-0.0808	C	4.3560	-0.8647	0.3577	H	5.0943	3.6852	0.1343
C	-1.6420	1.5715	-0.1338	C	3.4691	-1.8907	0.2985	H	5.8958	1.3424	0.3685
C	-2.5875	0.5121	0.0575	C	2.0860	2.0900	-0.0261	H	2.6991	-4.2546	-0.0021
C	-2.1447	-0.8255	0.2254	C	3.0157	3.1205	-0.0160	H	1.1513	-6.1294	-0.5332
C	-3.9624	0.8267	0.1384	C	4.3821	2.8535	0.1260	H	-1.2537	-5.6564	-0.9626
C	-4.8864	-0.1705	0.4776	C	4.8270	1.5562	0.2549	H	-2.1389	-3.3801	-0.7189

Table 3.528: Table of thermodynamic data as a function of temperature for Dibenz[*a,ghi*]naphtho[2,1,8-*cde*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	–55.492	501.195	501.195	∞
100	116.532	357.423	843.086	–48.566	528.084	575.970	–300.850
200	243.338	475.155	629.437	–30.856	513.810	629.563	–164.422
250	315.645	537.175	604.744	–16.892	507.134	659.273	–137.745
298.15	385.808	598.787	598.787	0.000	501.195	689.128	–120.730
300	388.469	601.182	598.794	0.716	500.975	690.292	–120.188
350	458.433	666.372	603.783	21.906	495.501	722.291	–107.794
400	523.351	731.889	615.702	46.475	490.749	755.011	–98.592
450	582.204	796.990	632.235	74.140	486.630	788.297	–91.501
500	634.825	861.109	651.927	104.591	483.050	822.035	–85.876
600	722.988	984.966	697.202	172.658	477.189	890.413	–77.516
700	792.483	1101.842	746.746	248.567	472.857	959.653	–71.609
800	847.948	1211.418	798.057	330.689	469.883	1029.402	–67.212
900	892.901	1313.977	849.747	417.807	468.090	1099.443	–63.809
1000	929.840	1410.027	901.024	509.003	467.317	1169.643	–61.095
1100	960.538	1500.133	951.436	603.568	467.362	1239.891	–58.876
1200	986.286	1584.847	1000.726	700.946	468.084	1310.082	–57.025
1300	1008.053	1664.676	1048.758	800.692	469.295	1380.206	–55.456
1400	1026.581	1740.076	1095.470	902.448	470.859	1450.226	–54.107
1500	1042.450	1811.458	1140.845	1005.920	472.699	1520.127	–52.934
1600	1056.121	1879.184	1184.893	1110.865	474.676	1589.889	–51.903
1700	1067.962	1943.574	1227.643	1217.083	476.718	1659.499	–50.989
1800	1078.270	2004.916	1269.134	1324.407	478.745	1729.062	–50.175
1900	1087.288	2063.462	1309.412	1432.695	480.729	1798.452	–49.442
2000	1095.213	2119.438	1348.524	1541.828	482.615	1867.770	–48.780
2100	1102.207	2173.047	1386.520	1651.706	484.317	1936.982	–48.179
2200	1108.407	2224.467	1423.448	1762.243	485.838	2006.119	–47.630
2300	1113.923	2273.862	1459.355	1873.365	487.175	2075.192	–47.128
2400	1118.850	2321.376	1494.289	1985.008	488.251	2144.155	–46.665
2500	1123.267	2367.141	1528.294	2097.118	489.080	2213.208	–46.242
2600	1127.238	2411.275	1561.411	2209.647	489.625	2282.099	–45.847
2700	1130.822	2453.886	1593.681	2322.553	489.891	2351.062	–45.483
2800	1134.065	2495.071	1625.142	2435.800	489.850	2420.040	–45.145
2900	1137.008	2534.919	1655.830	2549.356	489.470	2488.966	–44.830
3000	1139.687	2573.511	1685.780	2663.192	488.803	2557.943	–44.537
3100	1142.131	2610.921	1715.023	2777.285	487.760	2626.855	–44.261
3200	1144.366	2647.218	1743.590	2891.612	486.390	2695.893	–44.005
3300	1146.416	2682.464	1771.509	3006.152	484.675	2765.027	–43.766
3400	1148.300	2716.716	1798.808	3120.889	482.580	2834.114	–43.540
3500	1150.035	2750.028	1825.512	3235.807	480.114	2903.247	–43.328
3600	1151.636	2782.448	1851.645	3350.892	477.303	2972.562	–43.130
3700	1153.117	2814.023	1877.231	3466.130	474.109	3041.974	–42.944
3800	1154.488	2844.793	1902.290	3581.512	470.506	3111.413	–42.768
3900	1155.761	2874.798	1926.843	3697.025	466.540	3180.886	–42.602
4000	1156.944	2904.074	1950.909	3812.661	462.191	3250.631	–42.448
4100	1158.046	2932.656	1974.507	3928.411	457.422	3320.403	–42.302
4200	1159.074	2960.574	1997.653	4044.268	452.262	3390.287	–42.164
4300	1160.034	2987.859	2020.365	4160.224	446.698	3460.193	–42.032
4400	1160.932	3014.538	2042.658	4276.272	440.739	3530.338	–41.910
4500	1161.773	3040.637	2064.547	4392.408	434.403	3600.687	–41.795
4600	1162.562	3066.180	2086.045	4508.625	427.628	3671.196	–41.687
4700	1163.302	3091.191	2107.166	4624.919	420.433	3741.722	–41.584
4800	1163.999	3115.690	2127.922	4741.284	412.871	3812.530	–41.488
4900	1164.655	3139.697	2148.326	4857.717	404.856	3883.340	–41.396
5000	1165.273	3163.233	2168.390	4974.214	396.496	3954.533	–41.312

3.529. Dibenzo[*a,cd*]naphtho[8,1,2,3-*fghi*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 75459-08-4
Point Group: C₁

Length: 13.79 Å
Width: 12.80 Å
Breadth: 5.064 Å
L/B Ratio: 1.077

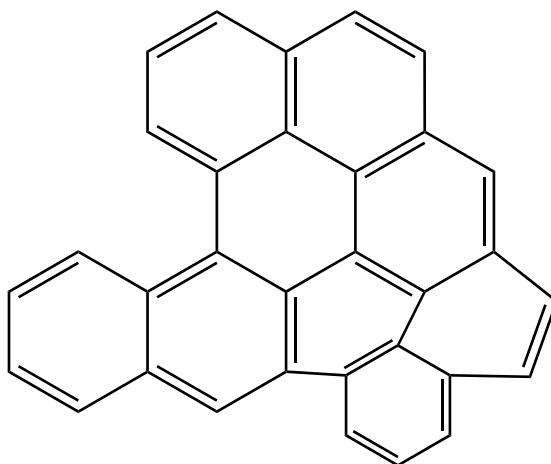
Cartesian coordinates:

C	1.0837	-0.8868	0.0148	C	-3.4519	3.7455	-0.1666	H	4.0476	2.9813	0.4886
C	2.3483	1.6724	0.1956	C	-4.0647	2.5228	-0.2735	H	2.6591	5.0386	0.6779
C	2.9514	2.9238	0.4107	C	-1.8934	1.4120	-0.0811	H	0.1858	4.9010	0.4219
C	2.1839	4.0671	0.5076	C	-3.2965	1.3325	-0.2252	H	2.8549	-2.8142	-0.8380
C	0.7985	3.9876	0.3742	C	-3.9254	0.0640	-0.3079	H	5.2851	-2.5748	-1.0984
C	0.3214	0.2775	0.0260	C	-1.1156	0.2183	-0.0383	H	6.4013	-0.4087	-0.5839
C	0.9470	1.5762	0.1191	C	0.4112	-2.1590	0.1949	H	5.0218	1.5661	0.0427
C	0.1720	2.7606	0.1782	C	-0.9605	-4.6243	0.4403	H	-1.5773	4.8168	0.0817
C	3.1472	0.4833	-0.0184	C	0.4111	-4.5476	0.6772	H	-4.0421	4.6672	-0.2001
C	2.5212	-0.7676	-0.1828	C	1.0797	-3.3443	0.5571	H	-5.1516	2.4502	-0.3937
C	3.3236	-1.8466	-0.6122	C	-1.6715	-3.4668	0.1477	H	-5.0153	0.0173	-0.4246
C	4.6875	-1.7204	-0.7636	C	-0.9969	-2.2206	0.0701	H	-1.4764	-5.5890	0.5030
C	5.3140	-0.4983	-0.4938	C	-1.7596	-1.0207	-0.0838	H	0.9623	-5.4507	0.9603
C	4.5479	0.5892	-0.1387	C	-3.1822	-1.0904	-0.2242	H	2.1604	-3.3214	0.7530
C	-1.2769	2.6899	0.0286	C	-3.8176	-2.3899	-0.2502	H	-4.9009	-2.4261	-0.4133
C	-2.0573	3.8304	-0.0110	C	-3.1014	-3.5154	-0.0635	H	-3.5829	-4.5002	-0.0645

Table 3.529: Table of thermodynamic data as a function of temperature for Dibenz[a,cd]naphtho[8,1,2,3-fghi]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	–55.444	512.862	512.862	∞
100	116.311	356.550	842.080	–48.553	539.765	587.738	–306.996
200	243.294	474.235	628.480	–30.849	525.485	641.422	–167.519
250	315.563	536.241	603.794	–16.888	518.806	671.178	–140.232
298.15	385.720	597.837	597.837	0.000	512.862	701.079	–122.824
300	388.381	600.232	597.845	0.716	512.642	702.245	–122.269
350	458.356	665.409	602.832	21.902	507.164	734.291	–109.585
400	523.291	730.917	614.750	46.467	502.409	767.060	–100.166
450	582.156	796.012	631.280	74.129	498.287	800.394	–92.905
500	634.788	860.126	650.969	104.578	494.704	834.181	–87.145
600	722.962	983.978	696.240	172.643	488.841	902.657	–78.582
700	792.464	1100.850	745.780	248.549	484.507	971.997	–72.530
800	847.931	1210.424	797.088	330.669	481.531	1041.845	–68.024
900	892.886	1312.981	848.774	417.786	479.736	1111.985	–64.537
1000	929.826	1409.029	900.049	508.980	478.962	1182.285	–61.755
1100	960.524	1499.135	950.459	603.543	479.006	1252.633	–59.481
1200	986.273	1583.847	999.747	700.920	479.726	1322.924	–57.584
1300	1008.041	1663.674	1047.778	800.666	480.936	1393.148	–55.976
1400	1026.570	1739.075	1094.488	902.421	482.499	1463.268	–54.594
1500	1042.440	1810.456	1139.861	1005.891	484.337	1533.270	–53.392
1600	1056.112	1878.180	1183.908	1110.835	486.313	1603.132	–52.336
1700	1067.953	1942.570	1226.657	1217.053	488.355	1672.843	–51.399
1800	1078.262	2003.911	1268.147	1324.375	490.381	1742.505	–50.565
1900	1087.280	2062.457	1308.424	1432.662	492.364	1811.996	–49.814
2000	1095.205	2118.433	1347.536	1541.795	494.249	1881.415	–49.136
2100	1102.200	2172.041	1385.530	1651.672	495.950	1950.727	–48.521
2200	1108.400	2223.461	1422.457	1762.208	497.470	2019.964	–47.959
2300	1113.917	2272.856	1458.365	1873.329	498.807	2089.139	–47.445
2400	1118.845	2320.370	1493.298	1984.972	499.882	2158.201	–46.971
2500	1123.261	2366.134	1527.302	2097.081	500.711	2227.356	–46.537
2600	1127.233	2410.268	1560.418	2209.609	501.255	2296.347	–46.133
2700	1130.817	2452.879	1592.688	2322.515	501.521	2365.411	–45.761
2800	1134.060	2494.063	1624.148	2435.761	501.480	2434.490	–45.415
2900	1137.004	2533.911	1654.836	2549.317	501.099	2503.517	–45.092
3000	1139.683	2572.503	1684.785	2663.153	500.431	2572.594	–44.792
3100	1142.127	2609.914	1714.028	2777.246	499.388	2641.607	–44.510
3200	1144.363	2646.210	1742.594	2891.572	498.018	2710.746	–44.247
3300	1146.413	2681.456	1770.513	3006.112	496.302	2779.981	–44.003
3400	1148.297	2715.708	1797.812	3120.849	494.207	2849.168	–43.771
3500	1150.032	2749.020	1824.515	3235.767	491.741	2918.402	–43.554
3600	1151.633	2781.440	1850.648	3350.851	488.929	2987.818	–43.351
3700	1153.114	2813.014	1876.233	3466.089	485.735	3057.330	–43.161
3800	1154.486	2843.784	1901.292	3581.470	482.132	3126.870	–42.981
3900	1155.759	2873.789	1925.845	3696.983	478.165	3196.445	–42.811
4000	1156.942	2903.066	1949.911	3812.619	473.817	3266.290	–42.652
4100	1158.044	2931.647	1973.509	3928.369	469.047	3336.163	–42.502
4200	1159.072	2959.566	1996.655	4044.225	463.887	3406.148	–42.361
4300	1160.032	2986.851	2019.367	4160.181	458.323	3476.155	–42.226
4400	1160.930	3013.530	2041.659	4276.229	452.363	3546.401	–42.100
4500	1161.771	3039.629	2063.547	4392.365	446.027	3616.850	–41.982
4600	1162.560	3065.172	2085.045	4508.582	439.252	3687.460	–41.872
4700	1163.301	3090.182	2106.166	4624.875	432.057	3758.087	–41.766
4800	1163.997	3114.681	2126.922	4741.240	424.494	3828.996	–41.667
4900	1164.653	3138.688	2147.327	4857.673	416.479	3899.907	–41.573
5000	1165.272	3162.224	2167.390	4974.170	408.120	3971.201	–41.486

3.530. Benzo[*e*]phenanthro[2,3,4,5-*pqrab*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-06-8
Point Group: C₁

Length: 14.16 Å
Width: 12.76 Å
Breadth: 4.942 Å
L/B Ratio: 1.110

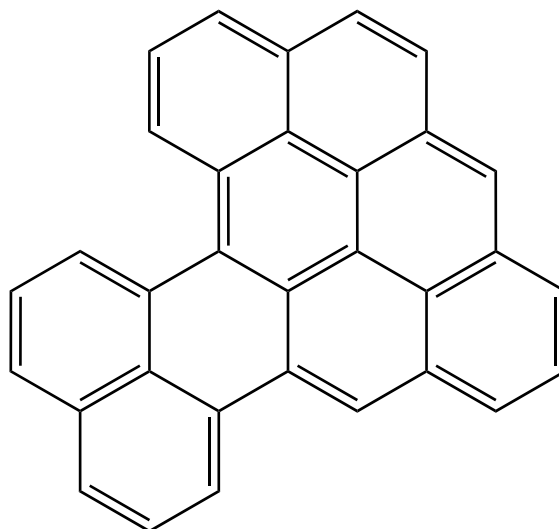
Cartesian coordinates:

C	1.9684	1.8418	0.1882	C	-2.3024	1.6997	-0.1248	H	5.8732	1.9514	0.1856
C	4.7778	1.9209	0.1900	C	-1.6243	2.9322	0.0077	H	4.5585	4.0437	0.4590
C	4.0456	3.0836	0.3396	C	-2.3335	4.1610	-0.0908	H	2.0760	3.9794	0.4423
C	2.6504	3.0466	0.3344	C	-3.6669	4.1705	-0.3924	H	4.7886	-2.6484	-0.3902
C	4.1185	0.6895	0.0423	C	-4.3354	2.9496	-0.6276	H	5.9555	-0.4719	-0.1387
C	2.7101	0.6463	0.0528	C	-3.6741	1.7581	-0.4987	H	2.7305	-3.9459	-0.4692
C	4.2248	-1.7175	-0.2591	C	-2.2090	-0.8267	0.2112	H	0.2920	3.9223	0.3085
C	4.8611	-0.5315	-0.1235	C	-3.5475	-0.9828	0.5888	H	-1.7883	5.0986	0.0677
C	2.7878	-1.7956	-0.2284	C	-4.1401	-2.2369	0.6772	H	-4.2201	5.1119	-0.4702
C	2.0322	-0.6141	-0.0721	C	-3.4114	-3.3826	0.3995	H	-5.3901	2.9672	-0.9217
C	2.1388	-3.0311	-0.3397	C	-1.4373	-2.0042	0.0484	H	-4.2155	0.8245	-0.7038
C	0.6217	-0.6723	-0.0284	C	-2.0507	-3.2768	0.0978	H	-4.1592	-0.1011	0.8239
C	-1.5689	0.4753	0.0506	C	-1.2596	-4.4587	-0.1399	H	-5.1930	-2.3172	0.9678
C	-0.1688	0.5333	0.0644	C	0.0757	-4.3774	-0.3231	H	-3.8896	-4.3678	0.4370
C	0.5096	1.7916	0.1479	C	0.7518	-3.1051	-0.2672	H	-1.7760	-5.4254	-0.1615
C	-0.2217	2.9549	0.1856	C	-0.0141	-1.9227	-0.1049	H	0.6795	-5.2742	-0.5033

Table 3.530: Table of thermodynamic data as a function of temperature for Benzo[*e*]phenanthro[2,3,4,5-*pqrab*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298 \text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-55.547	502.804	502.804	∞
100	116.531	359.235	845.204	-48.597	529.663	577.367	-301.579
200	243.487	477.015	631.412	-30.879	515.396	630.777	-164.739
250	315.884	539.079	606.700	-16.905	508.730	660.393	-137.979
298.15	386.106	600.738	600.738	0.000	502.804	690.156	-120.910
300	388.769	603.135	600.745	0.717	502.584	691.316	-120.366
350	458.754	668.373	605.738	21.922	497.126	723.216	-107.932
400	523.665	733.933	617.666	46.507	492.390	755.835	-98.700
450	582.495	799.070	634.210	74.187	488.287	789.017	-91.585
500	635.092	863.218	653.913	104.652	484.720	822.651	-85.940
600	723.215	987.120	699.213	172.744	478.884	890.815	-77.551
700	792.690	1104.029	748.780	248.674	474.574	959.838	-71.623
800	848.148	1213.632	800.112	330.816	471.620	1029.367	-67.209
900	893.100	1316.214	851.820	417.955	469.846	1099.185	-63.794
1000	930.038	1412.285	903.115	509.170	469.093	1169.160	-61.069
1100	960.733	1502.411	953.543	603.754	469.158	1239.182	-58.843
1200	986.478	1587.141	1002.848	701.152	469.899	1309.144	-56.984
1300	1008.239	1666.985	1050.894	800.917	471.129	1379.038	-55.409
1400	1026.760	1742.399	1097.619	902.692	472.711	1448.826	-54.055
1500	1042.621	1813.793	1143.006	1006.181	474.569	1518.495	-52.878
1600	1056.284	1881.529	1187.065	1111.143	476.562	1588.023	-51.843
1700	1068.116	1945.929	1229.825	1217.377	478.620	1657.398	-50.925
1800	1078.416	2007.279	1271.327	1324.715	480.663	1726.725	-50.107
1900	1087.425	2065.833	1311.614	1433.017	482.661	1795.878	-49.371
2000	1095.342	2121.816	1350.734	1542.164	484.559	1864.959	-48.707
2100	1102.329	2175.431	1388.738	1652.054	486.274	1933.933	-48.103
2200	1108.522	2226.857	1425.674	1762.603	487.807	2002.830	-47.552
2300	1114.032	2276.257	1461.589	1873.736	489.156	2071.665	-47.048
2400	1118.952	2323.775	1496.529	1985.390	490.241	2140.387	-46.583
2500	1123.363	2369.544	1530.540	2097.510	491.081	2209.201	-46.158
2600	1127.329	2413.682	1563.664	2210.048	491.635	2277.851	-45.762
2700	1130.908	2456.296	1595.939	2322.962	491.910	2346.573	-45.396
2800	1134.146	2497.484	1627.406	2436.218	491.877	2415.310	-45.057
2900	1137.085	2537.335	1658.099	2549.782	491.505	2483.995	-44.741
3000	1139.759	2575.929	1688.054	2663.626	490.845	2552.730	-44.446
3100	1142.200	2613.342	1717.302	2777.726	489.809	2621.400	-44.169
3200	1144.432	2649.641	1745.873	2892.059	488.446	2690.196	-43.912
3300	1146.478	2684.889	1773.796	3006.606	486.737	2759.087	-43.672
3400	1148.359	2719.143	1801.099	3121.349	484.649	2827.931	-43.445
3500	1150.091	2752.457	1827.807	3236.273	482.188	2896.822	-43.232
3600	1151.690	2784.878	1853.944	3351.363	479.382	2965.894	-43.033
3700	1153.168	2816.454	1879.533	3466.607	476.194	3035.063	-42.847
3800	1154.537	2847.225	1904.596	3581.993	472.596	3104.259	-42.670
3900	1155.808	2877.232	1929.152	3697.511	468.634	3173.489	-42.503
4000	1156.989	2906.509	1953.221	3813.151	464.291	3242.990	-42.348
4100	1158.089	2935.092	1976.822	3928.906	459.526	3312.519	-42.201
4200	1159.115	2963.012	1999.972	4044.767	454.370	3382.159	-42.062
4300	1160.073	2990.297	2022.687	4160.727	448.810	3451.821	-41.930
4400	1160.969	3016.977	2044.982	4276.779	442.855	3521.723	-41.807
4500	1161.809	3043.077	2066.873	4392.919	436.522	3591.827	-41.692
4600	1162.596	3068.621	2088.373	4509.139	429.751	3662.092	-41.584
4700	1163.336	3093.632	2109.497	4625.436	422.560	3732.374	-41.480
4800	1164.031	3118.132	2130.256	4741.805	415.000	3802.938	-41.384
4900	1164.686	3142.140	2150.662	4858.241	406.989	3873.503	-41.291
5000	1165.303	3165.676	2170.728	4974.741	398.632	3944.452	-41.207

3.531. Dinaphtho[1,8-*ab*:8',1',2',3'-*fghi*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-95-2
Point Group: C₁

Length: 14.24 Å
Width: 12.69 Å
Breadth: 5.128 Å
L/B Ratio: 1.122

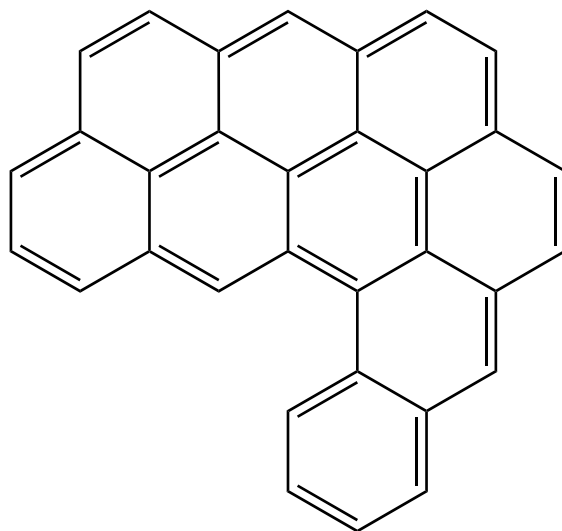
Cartesian coordinates:

C	2.2890	-1.6133	-0.2390	C	-4.1258	-0.4579	0.2073	H	-5.2832	1.9559	0.2531
C	0.8343	-1.6336	-0.1194	C	-1.2717	-2.8734	0.0037	H	-4.1049	4.1195	-0.0300
C	0.1320	-0.3644	-0.0193	C	-1.9509	-4.0823	0.0537	H	-5.2194	-0.4914	0.2860
C	0.8095	0.8478	0.0260	C	-3.3478	-4.1020	0.1650	H	-1.3962	-5.0261	0.0069
C	2.2604	0.8254	0.2466	C	-4.0656	-2.9274	0.2201	H	-3.8674	-5.0652	0.2067
C	2.9758	-0.3910	0.0100	C	0.6567	3.3151	-0.4361	H	-5.1580	-2.9471	0.3052
C	0.0588	2.0688	-0.1435	C	-0.0891	4.4667	-0.5608	H	-2.0563	5.3668	-0.4664
C	-1.3559	2.0304	-0.0771	C	-1.4773	4.4393	-0.3955	H	0.4066	5.4162	-0.7901
C	-2.0365	0.7846	0.0423	C	0.1606	-2.8149	-0.1168	H	1.7451	3.3741	-0.5742
C	-1.3020	-0.4058	0.0199	C	4.3860	-0.4059	0.0717	H	0.7154	-3.7619	-0.2203
C	-3.4672	0.7457	0.1371	C	5.0811	0.7598	0.4853	H	2.4559	2.8376	1.0013
C	-4.1940	1.9974	0.1366	C	4.3764	1.8770	0.8426	H	4.8959	2.7682	1.2103
C	-3.5532	3.1722	-0.0149	C	2.9725	1.9090	0.7223	H	6.1754	0.7408	0.5354
C	-2.1148	3.2311	-0.1625	C	3.0039	-2.7579	-0.5272	H	6.1897	-1.5789	-0.2340
C	-1.9937	-1.6519	0.0636	C	4.4123	-2.7412	-0.5579	H	4.9508	-3.6599	-0.8127
C	-3.4024	-1.6814	0.1664	C	5.0940	-1.5952	-0.2473	H	2.4640	-3.6993	-0.7120

Table 3.531: Table of thermodynamic data as a function of temperature for Dinaphtho[1,8-*ab*:8',1',2',3'-*fghi*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.534	538.722	538.722	∞
100	115.977	355.733	842.685	-48.695	565.483	613.537	-320.472
200	244.084	473.494	628.363	-30.974	551.220	667.305	-174.279
250	316.879	535.737	603.574	-16.959	544.595	697.092	-145.646
298.15	387.329	597.593	597.593	0.000	538.722	727.012	-127.367
300	389.998	599.997	597.600	0.719	538.505	728.178	-126.784
350	460.092	665.435	602.608	21.989	533.111	760.230	-113.456
400	525.030	731.175	614.571	46.642	528.444	792.991	-103.552
450	583.835	796.472	631.162	74.390	524.408	826.307	-95.913
500	636.378	860.759	650.918	104.921	520.907	860.067	-89.849
600	724.357	984.883	696.326	173.134	515.192	928.465	-80.828
700	793.684	1101.957	745.999	249.171	510.989	997.704	-74.448
800	849.008	1211.684	797.427	331.406	508.127	1067.433	-69.695
900	893.846	1314.361	849.223	418.624	506.434	1137.441	-66.014
1000	930.689	1410.505	900.596	509.909	505.751	1207.598	-63.077
1100	961.304	1500.689	951.094	604.555	505.877	1277.794	-60.676
1200	986.981	1585.466	1000.461	702.006	506.672	1347.927	-58.673
1300	1008.686	1665.347	1048.564	801.819	507.949	1417.986	-56.974
1400	1027.158	1740.793	1095.339	903.635	509.573	1487.936	-55.514
1500	1042.978	1812.213	1140.772	1007.162	511.468	1557.765	-54.245
1600	1056.605	1879.971	1184.872	1112.158	513.496	1627.449	-53.130
1700	1068.407	1944.390	1227.671	1218.422	515.584	1696.979	-52.141
1800	1078.680	2005.756	1269.207	1325.788	517.654	1766.459	-51.260
1900	1087.666	2064.323	1309.525	1434.115	519.677	1835.764	-50.468
2000	1095.562	2120.318	1348.675	1543.285	521.599	1904.995	-49.752
2100	1102.532	2173.943	1386.706	1653.197	523.335	1974.118	-49.102
2200	1108.708	2225.378	1423.667	1763.765	524.887	2043.164	-48.510
2300	1114.204	2274.786	1459.605	1874.916	526.254	2112.146	-47.967
2400	1119.112	2322.311	1494.567	1986.586	527.356	2181.016	-47.468
2500	1123.511	2368.087	1528.598	2098.721	528.211	2249.975	-47.010
2600	1127.467	2412.230	1561.740	2211.274	528.780	2318.771	-46.584
2700	1131.036	2454.849	1594.033	2324.202	529.068	2387.638	-46.191
2800	1134.266	2496.041	1625.516	2437.470	529.048	2456.519	-45.826
2900	1137.197	2535.896	1656.225	2551.045	528.687	2525.348	-45.485
3000	1139.865	2574.495	1686.194	2664.900	528.038	2594.227	-45.169
3100	1142.299	2611.911	1715.456	2779.010	527.012	2663.040	-44.871
3200	1144.525	2648.213	1744.040	2893.353	525.659	2731.979	-44.594
3300	1146.567	2683.464	1771.976	3007.909	523.959	2801.013	-44.335
3400	1148.443	2717.720	1799.291	3122.661	521.879	2870.000	-44.091
3500	1150.170	2751.036	1826.010	3237.593	519.427	2939.032	-43.862
3600	1151.765	2783.460	1852.157	3352.691	516.629	3008.246	-43.648
3700	1153.239	2815.038	1877.756	3467.942	513.448	3077.557	-43.446
3800	1154.605	2845.811	1902.828	3583.335	509.857	3146.894	-43.256
3900	1155.872	2875.819	1927.393	3698.860	505.902	3216.266	-43.076
4000	1157.050	2905.098	1951.471	3814.506	501.564	3285.908	-42.909
4100	1158.147	2933.682	1975.081	3930.267	496.805	3355.578	-42.750
4200	1159.170	2961.603	1998.238	4046.133	491.655	3425.359	-42.600
4300	1160.126	2988.890	2020.960	4162.099	486.101	3495.162	-42.457
4400	1161.020	3015.571	2043.263	4278.157	480.151	3565.204	-42.323
4500	1161.857	3041.672	2065.161	4394.301	473.823	3635.449	-42.198
4600	1162.643	3067.217	2086.668	4510.526	467.056	3705.854	-42.080
4700	1163.381	3092.229	2107.798	4626.828	459.870	3776.277	-41.968
4800	1164.074	3116.730	2128.563	4743.201	452.315	3846.981	-41.863
4900	1164.727	3140.739	2148.976	4859.641	444.307	3917.687	-41.762
5000	1165.343	3164.276	2169.047	4976.145	435.955	3988.775	-41.670

3.532. Dibenzo[*a,ghi*]naphtho[2,1,8-*lmn*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-04-6
Point Group: C₁

Length: 14.40 Å
Width: 12.56 Å
Breadth: 5.059 Å
L/B Ratio: 1.146

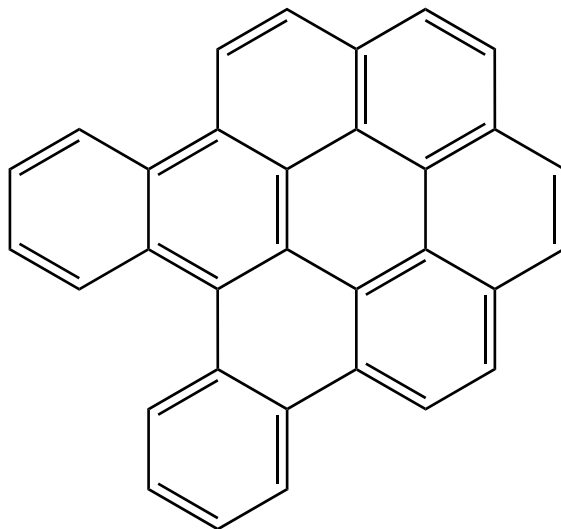
Cartesian coordinates:

C	5.0695	0.2042	-0.2551	C	0.8424	0.5043	-0.0588	H	6.1572	0.0908	-0.3276
C	4.4817	1.4081	-0.4113	C	0.2498	1.7939	-0.0964	H	5.0785	2.3052	-0.6133
C	3.0463	1.5665	-0.3129	C	-1.4315	-0.5412	0.0270	H	3.0640	3.7073	-0.5439
C	2.4542	2.8084	-0.3908	C	-4.2264	-0.1717	0.3211	H	1.0721	5.1146	-0.3524
C	1.0523	2.9426	-0.2470	C	-1.9821	0.7475	0.1508	H	-1.3718	5.3433	0.0206
C	0.4409	4.2283	-0.2207	C	-1.1586	1.9284	0.0773	H	2.0988	-4.1103	0.8223
C	-0.9030	4.3532	-0.0183	C	-1.7237	3.2029	0.1411	H	4.5711	-4.2986	0.7156
C	4.2861	-0.9787	0.0227	C	-3.1354	3.3470	0.3603	H	5.9682	-2.3169	0.2032
C	2.7114	-3.2307	0.5941	C	-3.9279	2.2553	0.4530	H	0.0818	-2.7736	0.5941
C	4.0869	-3.3329	0.5351	C	-3.3848	0.9287	0.3122	H	-5.3009	-0.0443	0.5034
C	4.8780	-2.2151	0.2468	C	-2.3227	-1.6375	-0.1639	H	-3.5488	4.3583	0.4477
C	2.0811	-1.9926	0.3575	C	-3.7145	-1.4487	0.0447	H	-5.0066	2.3538	0.6215
C	2.8736	-0.8616	0.0785	C	-4.6149	-2.5539	-0.0616	H	-5.6752	-2.3869	0.1608
C	2.2406	0.4030	-0.1095	C	-4.1665	-3.7819	-0.4432	H	-4.8494	-4.6332	-0.5271
C	0.6596	-1.8647	0.3710	C	-2.7953	-3.9592	-0.7574	H	-2.4568	-4.9357	-1.1196
C	0.0277	-0.6771	0.0986	C	-1.9129	-2.9286	-0.6212	H	-0.8592	-3.0891	-0.8880

Table 3.532: Table of thermodynamic data as a function of temperature for Dibenz[*a,ghi*]naphtho[2,1,8-*lmn*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.268	511.598	511.598	∞
100	114.911	355.390	839.963	-48.457	538.597	586.686	-306.447
200	242.876	472.284	626.591	-30.861	524.209	640.536	-167.287
250	315.745	534.266	601.887	-16.905	517.525	670.391	-140.068
298.15	386.207	595.924	595.924	0.000	511.598	700.386	-122.702
300	388.876	598.321	595.932	0.717	511.379	701.555	-122.149
350	458.954	663.585	600.926	21.931	505.929	733.695	-109.496
400	523.880	729.173	612.858	46.526	501.204	766.553	-100.099
450	582.694	794.334	629.409	74.216	497.111	799.972	-92.856
500	635.265	858.502	649.120	104.691	493.553	833.842	-87.109
600	723.350	982.432	694.435	172.798	487.733	902.476	-78.566
700	792.811	1099.361	744.017	248.741	483.435	971.967	-72.528
800	848.269	1208.980	795.361	330.895	480.493	1041.962	-68.032
900	893.227	1311.577	847.082	418.045	478.732	1112.245	-64.552
1000	930.171	1407.661	898.387	509.274	477.992	1182.683	-61.776
1100	960.871	1497.800	948.825	603.872	478.071	1253.166	-59.507
1200	986.617	1582.542	998.139	701.283	478.826	1323.590	-57.613
1300	1008.378	1662.397	1046.195	801.063	480.069	1393.942	-56.008
1400	1026.896	1737.822	1092.928	902.851	481.665	1464.189	-54.628
1500	1042.753	1809.225	1138.322	1006.354	483.536	1534.315	-53.428
1600	1056.411	1876.969	1182.389	1111.328	485.543	1604.300	-52.374
1700	1068.238	1941.377	1225.156	1217.575	487.613	1674.130	-51.439
1800	1078.532	2002.734	1266.664	1324.925	489.667	1743.911	-50.606
1900	1087.535	2061.294	1306.958	1433.238	491.677	1813.519	-49.856
2000	1095.446	2117.282	1346.084	1542.396	493.586	1883.054	-49.179
2100	1102.428	2170.902	1384.094	1652.296	495.311	1952.481	-48.564
2200	1108.615	2222.332	1421.035	1762.855	496.853	2021.831	-48.003
2300	1114.120	2271.736	1456.955	1873.997	498.211	2091.118	-47.490
2400	1119.036	2319.258	1491.900	1985.659	499.305	2160.292	-47.017
2500	1123.442	2365.030	1525.916	2097.787	500.153	2229.557	-46.583
2600	1127.404	2409.171	1559.043	2210.333	500.715	2298.659	-46.180
2700	1130.978	2451.788	1591.323	2323.255	500.997	2367.831	-45.808
2800	1134.213	2492.978	1622.794	2436.517	500.971	2437.019	-45.462
2900	1137.148	2532.831	1653.491	2550.087	500.606	2506.155	-45.140
3000	1139.819	2571.428	1683.449	2663.938	499.952	2575.339	-44.840
3100	1142.257	2608.843	1712.700	2778.043	498.922	2644.460	-44.558
3200	1144.486	2645.144	1741.275	2892.382	497.564	2713.706	-44.296
3300	1146.530	2680.393	1769.201	3006.934	495.861	2783.047	-44.051
3400	1148.408	2714.649	1796.507	3121.682	493.777	2852.340	-43.820
3500	1150.138	2747.964	1823.218	3236.611	491.321	2921.680	-43.603
3600	1151.734	2780.387	1849.358	3351.706	488.520	2991.201	-43.400
3700	1153.210	2811.964	1874.949	3466.954	485.336	3060.819	-43.210
3800	1154.578	2842.736	1900.014	3582.344	481.743	3130.464	-43.030
3900	1155.846	2872.743	1924.573	3697.866	477.785	3200.143	-42.860
4000	1157.026	2902.022	1948.644	3813.510	473.445	3270.093	-42.702
4100	1158.124	2930.606	1972.247	3929.269	468.683	3340.070	-42.552
4200	1159.149	2958.526	1995.399	4045.133	463.531	3410.159	-42.411
4300	1160.106	2985.813	2018.116	4161.096	457.975	3480.270	-42.276
4400	1161.000	3012.493	2040.413	4277.152	452.022	3550.620	-42.150
4500	1161.839	3038.594	2062.306	4393.294	445.693	3621.173	-42.033
4600	1162.625	3064.138	2083.808	4509.518	438.924	3691.886	-41.922
4700	1163.363	3089.150	2104.934	4625.818	431.736	3762.616	-41.816
4800	1164.058	3113.650	2125.694	4742.189	424.180	3833.628	-41.718
4900	1164.712	3137.659	2146.102	4858.628	416.170	3904.642	-41.623
5000	1165.328	3161.196	2166.170	4975.130	407.817	3976.039	-41.537

3.533. Dibenzo[*a,d*]coronene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-89-4
Point Group: C₂

Length: 13.71 Å
Width: 11.87 Å
Breadth: 5.078 Å
L/B Ratio: 1.155

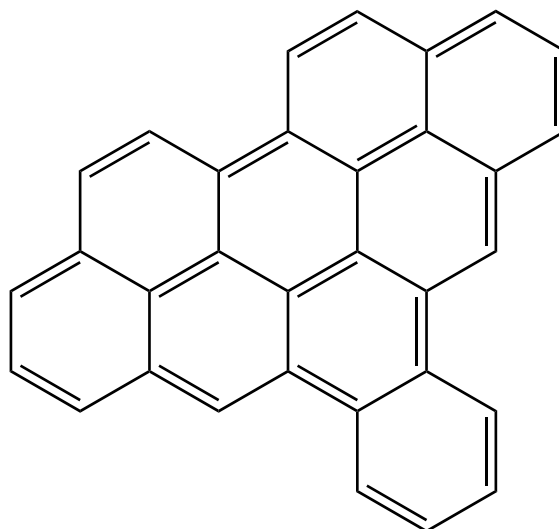
Cartesian coordinates:

C	1.6643	-0.0000	0.0000	C	-0.4649	-1.2350	0.0891	H	-2.4507	4.5771	-0.5630
C	0.2707	-0.0000	0.0000	C	0.2107	-2.4551	0.1590	H	0.0307	4.6018	-0.4300
C	0.2107	2.4550	-0.1591	C	-0.5268	-3.6561	0.3494	H	-5.8070	1.2137	-0.1676
C	-0.4649	1.2350	-0.0891	C	-1.8902	-3.6466	0.4179	H	-4.5674	3.3497	-0.4366
C	-1.8902	3.6466	-0.4179	C	1.6402	-2.4756	-0.0301	H	-4.5674	-3.3497	0.4366
C	-0.5267	3.6561	-0.3494	C	2.3500	-1.2663	-0.1800	H	-5.8070	-1.2137	0.1676
C	-2.6047	2.4260	-0.2887	C	3.7045	-1.3518	-0.5804	H	0.0307	-4.6018	0.4299
C	-1.8920	1.2271	-0.1321	C	4.3445	-2.5611	-0.7184	H	-2.4507	-4.5771	0.5630
C	-4.7111	1.2309	-0.1617	C	3.6557	-3.7562	-0.4629	H	4.2627	-0.4302	-0.7948
C	-4.0308	2.4027	-0.3076	C	2.3223	-3.7091	-0.1360	H	5.3930	-2.5973	-1.0319
C	-4.0100	0.0000	0.0000	C	2.3500	1.2663	0.1800	H	4.1781	-4.7148	-0.5429
C	-2.6098	-0.0000	0.0000	C	1.6402	2.4756	0.0301	H	1.7582	-4.6387	0.0353
C	-4.0308	-2.4027	0.3076	C	2.3222	3.7091	0.1359	H	1.7582	4.6387	-0.0353
C	-4.7111	-1.2309	0.1617	C	3.6557	3.7563	0.4629	H	4.1780	4.7149	0.5429
C	-2.6047	-2.4260	0.2887	C	4.3444	2.5612	0.7184	H	5.3930	2.5974	1.0319
C	-1.8920	-1.2271	0.1321	C	3.7044	1.3519	0.5804	H	4.2629	0.4304	0.7949

Table 3.533: Table of thermodynamic data as a function of temperature for Dibenzo[*a,d*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-55.589	485.522	485.522	∞
100	116.949	352.490	838.688	-48.620	512.358	560.737	-292.893
200	243.584	470.443	624.838	-30.879	498.115	614.810	-160.569
250	315.872	532.515	600.128	-16.903	491.451	644.754	-134.711
298.15	386.036	594.167	594.167	0.000	485.522	674.833	-118.226
300	388.697	596.563	594.174	0.717	485.303	676.006	-117.701
350	458.669	661.789	599.166	21.918	479.840	708.234	-105.696
400	523.593	727.338	611.091	46.499	475.101	741.183	-96.787
450	582.446	792.468	627.633	74.176	470.994	774.695	-89.922
500	635.063	856.612	647.333	104.639	467.425	808.659	-84.478
600	723.211	980.511	692.628	172.730	461.588	877.484	-76.390
700	792.686	1097.420	742.192	248.659	457.277	947.168	-70.677
800	848.131	1207.022	793.521	330.801	454.322	1017.358	-66.425
900	893.066	1309.601	845.227	417.936	452.546	1087.837	-63.135
1000	929.988	1405.667	896.520	509.147	451.789	1158.474	-60.511
1100	960.671	1495.787	946.945	603.726	451.848	1229.157	-58.367
1200	986.406	1580.512	996.248	701.117	452.583	1299.783	-56.577
1300	1008.162	1660.350	1044.292	800.875	453.805	1370.339	-55.060
1400	1026.680	1735.758	1091.014	902.642	455.380	1440.792	-53.755
1500	1042.540	1807.147	1136.398	1006.123	457.229	1511.125	-52.621
1600	1056.203	1874.877	1180.455	1111.077	459.214	1581.318	-51.624
1700	1068.037	1939.273	1223.213	1217.303	461.264	1651.358	-50.739
1800	1078.339	2000.618	1264.711	1324.633	463.299	1721.350	-49.951
1900	1087.351	2059.168	1304.996	1432.927	465.289	1791.170	-49.242
2000	1095.271	2115.148	1344.114	1542.067	467.181	1860.918	-48.601
2100	1102.261	2168.759	1382.115	1651.951	468.889	1930.559	-48.019
2200	1108.457	2220.182	1419.049	1762.493	470.415	2000.124	-47.488
2300	1113.970	2269.579	1454.961	1873.619	471.757	2069.626	-47.002
2400	1118.894	2317.095	1489.900	1985.267	472.837	2139.016	-46.554
2500	1123.307	2362.861	1523.909	2097.381	473.671	2208.498	-46.143
2600	1127.276	2406.997	1557.030	2209.914	474.220	2277.817	-45.761
2700	1130.857	2449.609	1589.304	2322.823	474.489	2347.207	-45.409
2800	1134.098	2490.795	1620.769	2436.074	474.452	2416.613	-45.082
2900	1137.039	2530.644	1651.460	2549.633	474.075	2485.967	-44.776
3000	1139.716	2569.237	1681.413	2663.473	473.411	2555.371	-44.492
3100	1142.158	2606.649	1710.659	2777.568	472.370	2624.710	-44.225
3200	1144.392	2642.947	1739.229	2891.897	471.003	2694.176	-43.977
3300	1146.441	2678.193	1767.151	3006.440	469.290	2763.737	-43.745
3400	1148.323	2712.446	1794.452	3121.180	467.198	2833.250	-43.527
3500	1150.057	2745.759	1821.159	3236.100	464.734	2902.811	-43.321
3600	1151.657	2778.180	1847.294	3351.187	461.925	2972.552	-43.130
3700	1153.137	2809.754	1872.882	3466.428	458.734	3042.391	-42.950
3800	1154.507	2840.525	1897.943	3581.811	455.133	3112.257	-42.780
3900	1155.779	2870.530	1922.498	3697.326	451.168	3182.157	-42.619
4000	1156.962	2899.807	1946.566	3812.964	446.821	3252.329	-42.470
4100	1158.063	2928.389	1970.166	3928.715	442.053	3322.528	-42.329
4200	1159.090	2956.308	1993.315	4044.574	436.896	3392.838	-42.195
4300	1160.049	2983.594	2016.028	4160.531	431.333	3463.170	-42.068
4400	1160.946	3010.273	2038.323	4276.581	425.375	3533.742	-41.950
4500	1161.786	3036.372	2060.213	4392.718	419.040	3604.517	-41.839
4600	1162.575	3061.916	2081.712	4508.937	412.267	3675.453	-41.735
4700	1163.315	3086.926	2102.834	4625.232	405.074	3746.406	-41.636
4800	1164.011	3111.425	2123.592	4741.598	397.512	3817.640	-41.544
4900	1164.667	3135.433	2143.998	4858.033	389.498	3888.876	-41.455
5000	1165.284	3158.969	2164.063	4974.530	381.140	3960.495	-41.374

3.534. Benzo[*h*]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-96-3
Point Group: C_{2v}

Length: 15.86 Å
Width: 12.91 Å
Breadth: 3.893 Å
L/B Ratio: 1.229

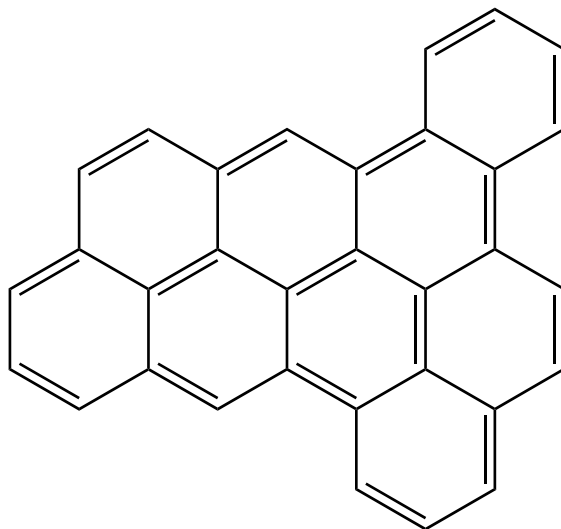
Cartesian coordinates:

C	4.9315	-2.1757	0.0000	C	-0.6830	2.8002	0.0000	H	5.4785	-3.1253	0.0000
C	5.6269	-0.9710	0.0000	C	0.7225	2.7903	0.0000	H	6.7221	-0.9781	0.0000
C	4.9470	0.2389	0.0000	C	1.4143	4.0094	0.0000	H	5.5037	1.1829	0.0000
C	3.5465	0.2616	0.0000	C	0.7334	5.2159	0.0000	H	3.3910	2.4396	0.0000
C	2.8205	1.4966	0.0000	C	-0.6594	5.2258	0.0000	H	-3.3562	2.4873	0.0000
C	1.4557	1.5248	0.0000	C	-1.3574	4.0291	0.0000	H	0.8594	-4.3385	0.0000
C	-1.4340	1.5453	0.0000	C	-3.5424	0.3117	0.0000	H	3.3440	-4.3557	0.0000
C	-2.7991	1.5363	0.0000	C	-4.9432	0.3088	0.0000	H	2.5151	3.9960	0.0000
C	-0.7006	0.3005	0.0000	C	-5.6401	-0.8913	0.0000	H	1.2891	6.1592	0.0000
C	0.7047	0.2906	0.0000	C	-4.9618	-2.1057	0.0000	H	-1.2017	6.1769	0.0000
C	1.3967	-0.9431	0.0000	C	-2.8426	-0.9158	0.0000	H	-2.4583	4.0314	0.0000
C	0.6887	-2.1680	0.0000	C	-3.5651	-2.1318	0.0000	H	-5.4864	1.2606	0.0000
C	1.4350	-3.4000	0.0000	C	-2.8350	-3.3721	0.0000	H	-6.7352	-0.8831	0.0000
C	2.7870	-3.4118	0.0000	C	-1.4830	-3.3794	0.0000	H	-5.5221	-3.0475	0.0000
C	3.5346	-2.1820	0.0000	C	-0.7193	-2.1580	0.0000	H	-3.4054	-4.3080	0.0000
C	2.8293	-0.9559	0.0000	C	-1.4099	-0.9233	0.0000	H	-0.9207	-4.3259	0.0000

Table 3.534: Table of thermodynamic data as a function of temperature for Benzo[*h*]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.688	492.778	492.778	∞
100	117.578	355.467	842.017	-48.655	519.579	567.660	-296.509
200	243.704	473.703	628.087	-30.877	505.373	621.416	-162.294
250	315.842	535.785	603.380	-16.899	498.711	651.196	-136.057
298.15	385.882	597.421	597.421	0.000	492.778	681.119	-119.327
300	388.539	599.816	597.428	0.716	492.558	682.285	-118.794
350	458.392	665.009	602.418	21.907	487.085	714.352	-106.609
400	523.220	730.514	614.336	46.471	482.329	747.141	-97.565
450	582.004	795.596	630.868	74.128	478.201	780.495	-90.596
500	634.581	859.691	650.555	104.568	474.609	814.304	-85.068
600	722.710	983.500	695.819	172.609	468.722	882.826	-76.855
700	792.219	1100.333	745.348	248.490	464.363	952.215	-71.054
800	847.717	1209.876	796.643	330.587	461.364	1022.116	-66.736
900	892.709	1312.410	848.317	417.684	459.550	1092.313	-63.395
1000	929.684	1408.442	899.579	508.862	458.760	1162.670	-60.730
1100	960.413	1498.535	949.978	603.413	458.791	1233.077	-58.553
1200	986.187	1583.239	999.256	700.780	459.502	1303.429	-56.736
1300	1007.975	1663.060	1047.277	800.518	460.703	1373.714	-55.195
1400	1026.520	1738.456	1093.980	902.267	462.261	1443.896	-53.871
1500	1042.402	1809.834	1139.345	1005.733	464.095	1513.960	-52.720
1600	1056.083	1877.557	1183.385	1110.674	466.068	1583.884	-51.707
1700	1067.932	1941.945	1226.128	1216.889	468.106	1653.657	-50.810
1800	1078.247	2003.285	1267.613	1324.210	470.131	1723.382	-50.010
1900	1087.270	2061.830	1307.885	1432.495	472.113	1792.935	-49.290
2000	1095.198	2117.806	1346.992	1541.627	473.997	1862.417	-48.640
2100	1102.196	2171.413	1384.983	1651.504	475.698	1931.792	-48.050
2200	1108.399	2222.834	1421.906	1762.040	477.217	2001.092	-47.511
2300	1113.917	2272.228	1457.810	1873.161	478.555	2070.329	-47.018
2400	1118.846	2319.742	1492.740	1984.804	479.629	2139.455	-46.563
2500	1123.263	2365.507	1526.741	2096.913	480.459	2208.672	-46.147
2600	1127.236	2409.641	1559.855	2209.442	481.003	2277.726	-45.759
2700	1130.821	2452.251	1592.123	2322.347	481.269	2346.852	-45.402
2800	1134.064	2493.436	1623.581	2435.594	481.228	2415.994	-45.070
2900	1137.008	2533.284	1654.267	2549.150	480.848	2485.084	-44.760
3000	1139.687	2571.876	1684.214	2662.987	480.181	2554.224	-44.472
3100	1142.131	2609.287	1713.455	2777.080	479.137	2623.299	-44.201
3200	1144.367	2645.584	1742.019	2891.406	477.768	2692.501	-43.950
3300	1146.418	2680.830	1769.937	3005.947	476.053	2761.798	-43.715
3400	1148.302	2715.082	1797.234	3120.684	473.958	2831.048	-43.493
3500	1150.037	2748.394	1823.936	3235.603	471.492	2900.345	-43.284
3600	1151.638	2780.814	1850.068	3350.687	468.681	2969.823	-43.090
3700	1153.119	2812.388	1875.652	3465.926	465.488	3039.398	-42.908
3800	1154.490	2843.159	1900.709	3581.307	461.885	3109.001	-42.735
3900	1155.763	2873.164	1925.261	3696.821	457.918	3178.638	-42.572
4000	1156.946	2902.440	1949.326	3812.457	453.571	3248.546	-42.421
4100	1158.048	2931.022	1972.922	3928.207	448.801	3318.482	-42.277
4200	1159.076	2958.940	1996.068	4044.064	443.642	3388.529	-42.142
4300	1160.036	2986.225	2018.779	4160.020	438.078	3458.598	-42.013
4400	1160.934	3012.905	2041.071	4276.069	432.119	3528.907	-41.893
4500	1161.775	3039.004	2062.958	4392.205	425.783	3599.419	-41.780
4600	1162.563	3064.547	2084.455	4508.422	419.008	3670.091	-41.674
4700	1163.304	3089.557	2105.575	4624.716	411.814	3740.781	-41.573
4800	1164.001	3114.056	2126.331	4741.082	404.251	3811.752	-41.479
4900	1164.657	3138.064	2146.734	4857.515	396.237	3882.725	-41.390
5000	1165.275	3161.599	2166.797	4974.012	387.877	3954.081	-41.307

3.535. Dinaphtho[2,1,8-*fgh*:7',8',1',2',3'-*pqrst*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-98-5
Point Group: C_s

Length: 15.88 Å
Width: 12.90 Å
Breadth: 3.890 Å
L/B Ratio: 1.231

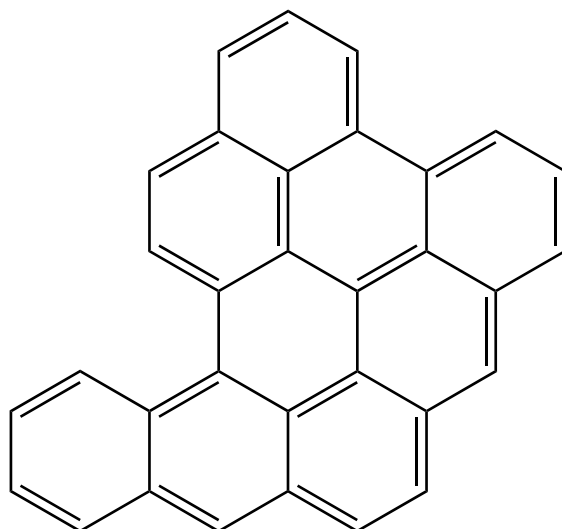
Cartesian coordinates:

C	0.0898	2.5046	0.0000	C	1.1520	1.5011	0.0000	H	1.4371	4.1780	0.0000
C	0.3840	3.8566	0.0000	C	2.4701	1.8647	0.0000	H	-0.3730	5.8815	0.0000
C	-0.6390	4.8193	0.0000	C	0.7851	0.1057	0.0000	H	-2.7597	5.1764	0.0000
C	-1.9561	4.4313	0.0000	C	-0.5715	-0.2967	0.0000	H	-4.4397	3.4025	0.0000
C	-1.2703	2.0851	0.0000	C	-0.8985	-1.6647	0.0000	H	-5.0214	0.9861	0.0000
C	-2.2913	3.0565	0.0000	C	0.1280	-2.6259	0.0000	H	-5.4417	-0.7375	0.0000
C	-3.6544	2.6379	0.0000	C	3.5171	0.8894	0.0000	H	-6.0354	-3.1523	0.0000
C	-3.9705	1.3137	0.0000	C	5.5309	-1.0639	0.0000	H	-4.2421	-4.8763	0.0000
C	-2.9554	0.3125	0.0000	C	5.8597	0.2916	0.0000	H	-1.8523	-4.1878	0.0000
C	-1.6176	0.6962	0.0000	C	4.8709	1.2612	0.0000	H	2.7426	2.9328	0.0000
C	-2.2920	-2.0676	0.0000	C	4.1957	-1.4626	0.0000	H	-0.1441	-3.6937	0.0000
C	-3.3054	-1.0932	0.0000	C	3.1761	-0.4801	0.0000	H	6.3251	-1.8190	0.0000
C	-4.6541	-1.5063	0.0000	C	1.7995	-0.8691	0.0000	H	6.9136	0.5897	0.0000
C	-4.9851	-2.8433	0.0000	C	1.4613	-2.2487	0.0000	H	5.1388	2.3238	0.0000
C	-3.9747	-3.8147	0.0000	C	2.5220	-3.2289	0.0000	H	2.2387	-4.2878	0.0000
C	-2.6517	-3.4312	0.0000	C	3.8202	-2.8564	0.0000	H	4.6229	-3.6028	0.0000

Table 3.535: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1,8-*fgh*:7',8',1',2',3'-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.564	481.734	481.734	∞
100	117.340	362.209	847.233	-48.502	508.687	556.094	-290.468
200	242.882	480.054	633.973	-30.784	494.422	609.195	-159.102
250	314.886	541.938	609.340	-16.851	487.715	638.663	-133.438
298.15	384.840	603.397	603.397	0.000	481.734	668.293	-117.080
300	387.494	605.786	603.404	0.714	481.512	669.448	-116.559
350	457.302	670.813	608.380	21.851	475.985	701.221	-104.649
400	522.122	736.172	620.270	46.361	471.174	733.723	-95.812
450	580.927	801.126	636.763	73.963	466.993	766.798	-89.006
500	633.543	865.109	656.409	104.350	463.348	800.333	-83.609
600	721.778	988.738	701.584	172.292	457.362	868.322	-75.593
700	791.398	1105.436	751.028	248.086	452.915	937.195	-69.933
800	846.999	1214.876	802.244	330.106	449.839	1006.591	-65.722
900	892.080	1317.331	853.846	417.136	447.957	1076.292	-62.465
1000	929.132	1413.300	905.045	508.255	447.109	1146.161	-59.868
1100	959.925	1503.344	955.386	602.754	447.088	1216.085	-57.746
1200	985.755	1588.008	1004.612	700.075	447.753	1285.957	-55.975
1300	1007.590	1667.797	1052.587	799.772	448.914	1355.767	-54.474
1400	1026.175	1743.165	1099.247	901.485	450.434	1425.477	-53.184
1500	1042.092	1814.521	1144.575	1004.918	452.236	1495.071	-52.062
1600	1055.803	1882.224	1188.581	1109.830	454.179	1564.528	-51.076
1700	1067.678	1946.597	1231.292	1216.018	456.191	1633.835	-50.201
1800	1078.016	2007.923	1272.748	1323.314	458.192	1703.096	-49.422
1900	1087.058	2066.456	1312.994	1431.578	460.151	1772.186	-48.720
2000	1095.005	2122.421	1352.076	1540.689	462.015	1841.205	-48.086
2100	1102.018	2176.020	1390.044	1650.548	463.697	1910.119	-47.511
2200	1108.234	2227.432	1426.947	1761.067	465.200	1978.959	-46.985
2300	1113.765	2276.819	1462.831	1872.172	466.521	2047.737	-46.505
2400	1118.705	2324.327	1497.744	1983.800	467.582	2116.403	-46.061
2500	1123.133	2370.086	1531.728	2095.896	468.397	2185.162	-45.656
2600	1127.114	2414.215	1564.826	2208.412	468.929	2253.759	-45.278
2700	1130.707	2456.821	1597.078	2321.306	469.183	2322.428	-44.929
2800	1133.958	2498.002	1628.523	2434.542	469.131	2391.112	-44.606
2900	1136.908	2537.846	1659.196	2548.087	468.741	2459.746	-44.304
3000	1139.593	2576.435	1689.131	2661.914	468.064	2528.430	-44.023
3100	1142.043	2613.843	1718.360	2775.998	467.012	2597.050	-43.759
3200	1144.284	2650.137	1746.913	2890.316	465.634	2665.796	-43.514
3300	1146.339	2685.381	1774.820	3004.849	463.910	2734.638	-43.285
3400	1148.228	2719.631	1802.108	3119.578	461.808	2803.433	-43.069
3500	1149.967	2752.941	1828.801	3234.489	459.335	2872.275	-42.865
3600	1151.571	2785.359	1854.924	3349.567	456.517	2941.298	-42.676
3700	1153.055	2816.931	1880.499	3464.800	453.317	3010.420	-42.499
3800	1154.430	2847.700	1905.548	3580.175	449.708	3079.568	-42.331
3900	1155.706	2877.703	1930.092	3695.682	445.736	3148.751	-42.172
4000	1156.892	2906.978	1954.150	3811.313	441.382	3218.205	-42.025
4100	1157.996	2935.559	1977.740	3927.058	436.608	3287.687	-41.885
4200	1159.026	2963.476	2000.879	4042.910	431.443	3357.280	-41.753
4300	1159.988	2990.760	2023.583	4158.861	425.875	3426.896	-41.628
4400	1160.888	3017.438	2045.869	4274.905	419.911	3496.752	-41.511
4500	1161.731	3043.536	2067.750	4391.037	413.570	3566.810	-41.402
4600	1162.522	3069.078	2089.241	4507.250	406.791	3637.029	-41.299
4700	1163.264	3094.088	2110.356	4623.540	399.593	3707.266	-41.201
4800	1163.963	3118.586	2131.106	4739.901	392.027	3777.784	-41.110
4900	1164.620	3142.593	2151.505	4856.331	384.008	3848.304	-41.023
5000	1165.240	3166.128	2171.563	4972.824	375.645	3919.208	-40.943

3.536. Pyreno[5,4,3,2,1-*pqrst*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-11-5
Point Group: C₁

Length: 15.86 Å
Width: 12.86 Å
Breadth: 4.951 Å
L/B Ratio: 1.234

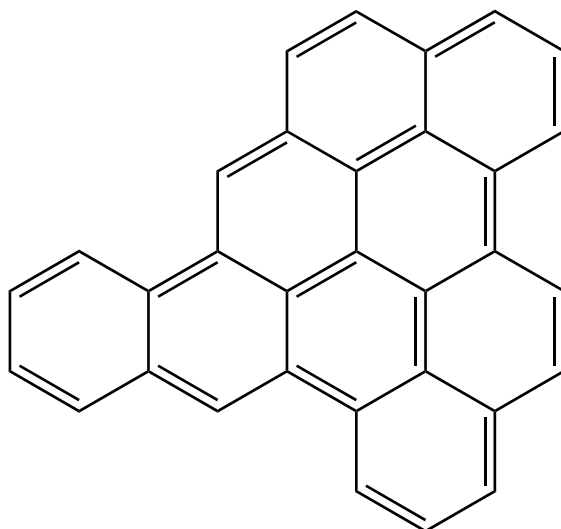
Cartesian coordinates:

C	2.3756	-4.0928	-0.2618	C	-0.7444	3.9401	-0.2938	H	-5.3040	-3.0290	1.0868
C	1.3520	-3.1220	-0.2886	C	0.3034	2.9541	-0.1247	H	-7.0033	-1.2966	0.5494
C	1.6633	-1.7606	-0.1069	C	-3.1770	-0.5127	0.1325	H	-6.2649	0.9849	-0.1185
C	3.0221	-1.3805	0.0668	C	-4.1499	0.4957	-0.0471	H	-2.9106	-2.5607	0.8322
C	4.0060	-2.3567	0.0973	C	-3.7561	1.8383	-0.2903	H	-4.5297	2.6013	-0.4435
C	3.6824	-3.7109	-0.0615	C	-5.5313	0.1939	0.0763	H	-2.8279	4.3133	-0.5167
C	0.6096	-0.7865	-0.0974	C	-5.9395	-1.0586	0.4506	H	-0.4494	4.9941	-0.3531
C	-0.7315	-1.1796	-0.1912	C	-4.9753	-2.0451	0.7359	H	1.8832	4.4033	0.0202
C	-0.9954	-2.5572	-0.4774	C	-3.6391	-1.7773	0.5828	H	4.2370	3.8341	0.3592
C	-0.0077	-3.4892	-0.5204	C	2.3214	0.9994	0.1088	H	6.0279	2.1201	0.5581
C	0.9558	0.6009	-0.0191	C	2.6460	2.3716	0.1523	H	5.4702	-0.3014	0.4193
C	-0.0509	1.5640	-0.1089	C	1.6133	3.3398	0.0156	H	-0.2363	-4.5384	-0.7409
C	-1.4245	1.1613	-0.1527	C	3.3610	0.0325	0.1886	H	-2.0287	-2.8674	-0.6849
C	-1.7829	-0.1948	-0.0714	C	4.6700	0.4518	0.3523	H	5.0547	-2.0544	0.2433
C	-2.4294	2.1790	-0.2740	C	4.9839	1.8183	0.4239	H	4.4801	-4.4603	-0.0309
C	-2.0337	3.5700	-0.3791	C	3.9947	2.7662	0.3175	H	2.1165	-5.1484	-0.4013

Table 3.536: Table of thermodynamic data as a function of temperature for Pyreno[5,4,3,2,1-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.501	512.786	512.786	∞
100	116.126	357.924	843.782	-48.586	539.656	587.492	-306.868
200	243.500	475.555	629.991	-30.887	525.371	641.044	-167.420
250	315.976	537.631	605.272	-16.910	518.708	670.732	-140.139
298.15	386.212	599.309	599.309	0.000	512.786	700.564	-122.733
300	388.874	601.706	599.316	0.717	512.567	701.727	-122.179
350	458.843	666.960	604.310	21.928	507.114	733.698	-109.496
400	523.729	732.530	616.240	46.516	502.382	766.388	-100.078
450	582.533	797.673	632.787	74.199	498.281	799.640	-92.818
500	635.108	861.823	652.493	104.665	494.715	833.344	-87.057
600	723.201	985.726	697.797	172.757	488.879	901.647	-78.494
700	792.660	1102.631	747.367	248.685	484.567	970.810	-72.441
800	848.111	1212.230	798.700	330.824	481.610	1040.479	-67.935
900	893.060	1314.807	850.410	417.958	479.832	1110.437	-64.447
1000	929.999	1410.874	901.705	509.169	479.076	1180.553	-61.665
1100	960.696	1500.996	952.132	603.750	479.136	1250.716	-59.390
1200	986.442	1585.723	1001.437	701.144	479.874	1320.820	-57.493
1300	1008.206	1665.564	1049.483	800.906	481.100	1390.856	-55.884
1400	1026.729	1740.976	1096.207	902.677	482.679	1460.786	-54.501
1500	1042.593	1812.368	1141.592	1006.163	484.534	1530.598	-53.299
1600	1056.258	1880.102	1185.651	1111.123	486.525	1600.268	-52.242
1700	1068.092	1944.501	1228.411	1217.354	488.580	1669.786	-51.305
1800	1078.394	2005.850	1269.911	1324.690	490.620	1739.255	-50.471
1900	1087.404	2064.402	1310.197	1432.990	492.616	1808.551	-49.720
2000	1095.323	2120.385	1349.317	1542.134	494.513	1877.776	-49.041
2100	1102.311	2173.998	1387.320	1652.023	496.225	1946.893	-48.425
2200	1108.505	2225.423	1424.255	1762.570	497.756	2015.934	-47.863
2300	1114.016	2274.822	1460.170	1873.702	499.104	2084.912	-47.349
2400	1118.938	2322.340	1495.110	1985.354	500.188	2153.778	-46.875
2500	1123.349	2368.109	1529.120	2097.472	501.026	2222.735	-46.441
2600	1127.317	2412.246	1562.242	2210.009	501.579	2291.529	-46.036
2700	1130.896	2454.859	1594.518	2322.923	501.853	2360.394	-45.664
2800	1134.135	2496.047	1625.984	2436.177	501.819	2429.275	-45.318
2900	1137.074	2535.897	1656.677	2549.740	501.446	2498.103	-44.995
3000	1139.749	2574.492	1686.631	2663.583	500.785	2566.982	-44.694
3100	1142.190	2611.904	1715.878	2777.682	499.748	2635.796	-44.412
3200	1144.423	2648.203	1744.449	2892.014	498.384	2704.736	-44.149
3300	1146.470	2683.451	1772.372	3006.560	496.674	2773.771	-43.904
3400	1148.351	2717.705	1799.674	3121.302	494.585	2842.759	-43.673
3500	1150.084	2751.018	1826.382	3236.225	492.124	2911.793	-43.455
3600	1151.683	2783.439	1852.519	3351.315	489.317	2981.009	-43.252
3700	1153.161	2815.015	1878.107	3466.558	486.128	3050.322	-43.062
3800	1154.531	2845.786	1903.169	3581.943	482.530	3119.661	-42.882
3900	1155.802	2875.792	1927.725	3697.461	478.567	3189.035	-42.711
4000	1156.983	2905.070	1951.794	3813.101	474.223	3258.681	-42.553
4100	1158.083	2933.652	1975.395	3928.855	469.457	3328.353	-42.403
4200	1159.109	2961.572	1998.544	4044.715	464.301	3398.137	-42.261
4300	1160.068	2988.857	2021.259	4160.674	458.740	3467.943	-42.126
4400	1160.964	3015.537	2043.554	4276.726	452.785	3537.989	-42.000
4500	1161.804	3041.637	2065.445	4392.865	446.451	3608.238	-41.882
4600	1162.592	3067.181	2086.945	4509.085	439.680	3678.647	-41.771
4700	1163.331	3092.192	2108.068	4625.382	432.488	3749.073	-41.665
4800	1164.027	3116.691	2128.826	4741.750	424.928	3819.781	-41.567
4900	1164.682	3140.699	2149.233	4858.186	416.916	3890.490	-41.472
5000	1165.299	3164.235	2169.298	4974.685	408.560	3961.583	-41.386

3.537. Dinaphtho[2,1,8-*fgh*:3',2',1',8',7'-*rstuv*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-93-0
Point Group: C_s

Length: 15.88 Å
Width: 12.88 Å
Breadth: 3.893 Å
L/B Ratio: 1.233

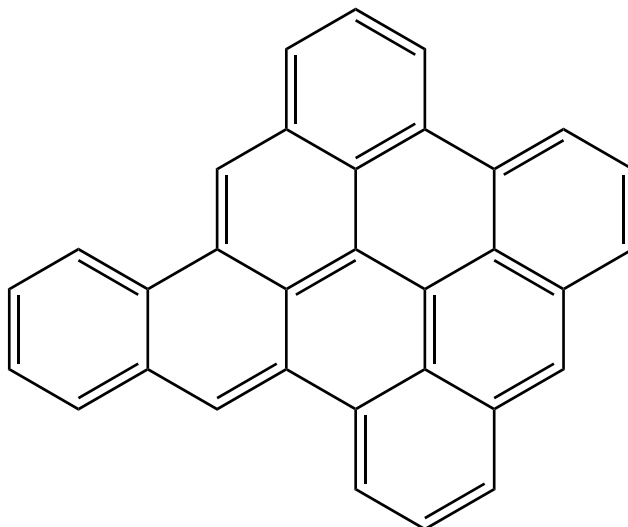
Cartesian coordinates:

C	3.1062	1.1843	0.0000	C	-3.2300	-0.2148	0.0000	H	3.6395	2.1491	0.0000
C	1.7683	-1.3040	0.0000	C	-4.6284	-0.2907	0.0000	H	1.6692	-3.4642	0.0000
C	1.0821	-2.5315	0.0000	C	-5.2720	-1.5194	0.0000	H	-3.1904	4.4195	0.0000
C	-2.5331	1.0558	0.0000	C	-4.5389	-2.7011	0.0000	H	-4.3632	2.2227	0.0000
C	-2.6235	3.4816	0.0000	C	-2.4793	-1.4109	0.0000	H	2.6931	3.6834	0.0000
C	-3.2636	2.2796	0.0000	C	-3.1434	-2.6597	0.0000	H	1.3732	5.7886	0.0000
C	-1.1988	3.5429	0.0000	C	-2.3617	-3.8732	0.0000	H	-1.1140	5.7123	0.0000
C	1.5930	3.6382	0.0000	C	-1.0122	-3.8339	0.0000	H	-5.2102	0.6438	0.0000
C	0.8466	4.8286	0.0000	C	-0.3029	-2.5763	0.0000	H	-6.3664	-1.5590	0.0000
C	-0.5258	4.7877	0.0000	C	-1.0455	-1.3655	0.0000	H	-5.0549	-3.6679	0.0000
C	0.9665	2.4046	0.0000	C	3.8707	-0.0239	0.0000	H	-2.8994	-4.8284	0.0000
C	-0.4556	2.3455	0.0000	C	3.2140	-1.2669	0.0000	H	-0.4194	-4.7559	0.0000
C	-1.1411	1.0900	0.0000	C	3.9867	-2.4488	0.0000	H	3.4635	-3.4172	0.0000
C	-0.3747	-0.1327	0.0000	C	5.3609	-2.3882	0.0000	H	5.9541	-3.3085	0.0000
C	1.0398	-0.0965	0.0000	C	6.0146	-1.1439	0.0000	H	7.1089	-1.1105	0.0000
C	1.7401	1.1640	0.0000	C	5.2832	0.0210	0.0000	H	5.7865	0.9945	0.0000

Table 3.537: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1,8-*fgh*:3',2',1',8',7'-*rstuv*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.685	481.956	481.956	∞
100	117.771	362.337	848.443	-48.611	508.801	556.196	-290.521
200	243.441	480.559	634.744	-30.837	494.591	609.263	-159.120
250	315.422	542.565	610.070	-16.876	487.912	638.702	-133.447
298.15	385.381	604.119	604.119	0.000	481.956	668.300	-117.081
300	388.036	606.511	604.126	0.715	481.735	669.454	-116.560
350	457.860	671.623	609.109	21.880	476.236	701.188	-104.644
400	522.691	737.057	621.014	46.418	471.454	733.648	-95.803
450	581.497	802.078	637.526	74.048	467.300	766.677	-88.992
500	634.104	866.121	657.194	104.464	463.684	800.163	-83.591
600	722.302	989.849	702.415	172.460	457.752	868.046	-75.569
700	791.877	1106.625	751.905	248.304	453.356	936.803	-69.904
800	847.433	1216.126	803.164	330.370	450.326	1006.078	-65.689
900	892.473	1318.629	854.806	417.441	448.485	1075.651	-62.428
1000	929.486	1414.638	906.040	508.597	447.673	1145.388	-59.828
1100	960.247	1504.714	956.414	603.130	447.686	1215.176	-57.703
1200	986.047	1589.405	1005.670	700.482	448.382	1284.911	-55.930
1300	1007.855	1669.215	1053.672	800.207	449.571	1354.579	-54.427
1400	1026.417	1744.603	1100.357	901.945	451.117	1424.146	-53.134
1500	1042.313	1815.974	1145.707	1005.401	452.941	1493.596	-52.011
1600	1056.006	1883.692	1189.733	1110.334	454.906	1562.907	-51.023
1700	1067.864	1948.076	1232.463	1216.542	456.937	1632.066	-50.146
1800	1078.187	2009.412	1273.937	1323.856	458.956	1701.179	-49.366
1900	1087.216	2067.954	1314.198	1432.136	460.932	1770.119	-48.663
2000	1095.150	2123.927	1353.296	1541.262	462.810	1838.989	-48.028
2100	1102.153	2177.532	1391.278	1651.135	464.507	1907.752	-47.452
2200	1108.359	2228.951	1428.193	1761.667	466.022	1976.440	-46.926
2300	1113.881	2278.343	1464.089	1872.784	467.356	2045.065	-46.444
2400	1118.813	2325.856	1499.013	1984.423	468.427	2113.580	-46.000
2500	1123.234	2371.619	1533.007	2096.529	469.253	2182.185	-45.593
2600	1127.209	2415.752	1566.115	2209.055	469.795	2250.629	-45.215
2700	1130.795	2458.362	1598.377	2321.958	470.058	2319.143	-44.866
2800	1134.041	2499.546	1629.830	2435.203	470.015	2387.674	-44.542
2900	1136.986	2539.393	1660.511	2548.756	469.632	2456.153	-44.239
3000	1139.667	2577.984	1690.454	2662.591	468.963	2524.682	-43.958
3100	1142.113	2615.394	1719.690	2776.682	467.918	2593.147	-43.693
3200	1144.350	2651.691	1748.251	2891.007	466.547	2661.738	-43.448
3300	1146.401	2686.936	1776.165	3005.546	464.830	2730.425	-43.218
3400	1148.286	2721.188	1803.458	3120.281	462.733	2799.064	-43.001
3500	1150.022	2754.499	1830.157	3235.198	460.266	2867.750	-42.798
3600	1151.624	2786.919	1856.285	3350.281	457.453	2936.618	-42.608
3700	1153.106	2818.493	1881.866	3465.519	454.259	3005.583	-42.430
3800	1154.478	2849.263	1906.921	3580.899	450.655	3074.575	-42.262
3900	1155.751	2879.268	1931.470	3696.411	446.687	3143.601	-42.103
4000	1156.935	2908.544	1955.532	3812.046	442.338	3212.899	-41.955
4100	1158.038	2937.125	1979.126	3927.795	437.567	3282.224	-41.815
4200	1159.066	2965.044	2002.269	4043.651	432.407	3351.661	-41.683
4300	1160.026	2992.328	2024.978	4159.606	426.842	3421.120	-41.558
4400	1160.925	3019.007	2047.268	4275.654	420.882	3490.819	-41.440
4500	1161.766	3045.106	2069.153	4391.789	414.545	3560.720	-41.331
4600	1162.555	3070.649	2090.648	4508.006	407.770	3630.782	-41.228
4700	1163.296	3095.659	2111.766	4624.299	400.575	3700.862	-41.130
4800	1163.993	3120.158	2132.520	4740.664	393.012	3771.223	-41.038
4900	1164.650	3144.166	2152.921	4857.096	384.996	3841.586	-40.951
5000	1165.268	3167.701	2172.982	4973.592	376.636	3912.332	-40.871

3.538. Benzo[*e*]phenanthro[1,10,9,8-*opqra*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-99-6
Point Group: C_s

Length: 15.90 Å
Width: 12.89 Å
Breadth: 3.891 Å
L/B Ratio: 1.234

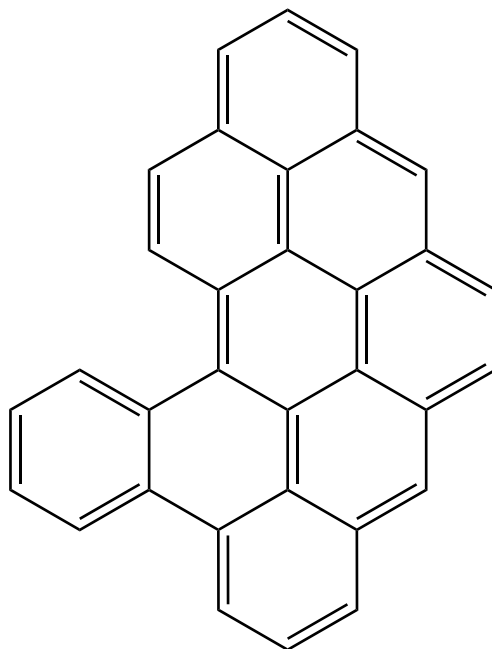
Cartesian coordinates:

C	2.7205	1.7809	0.0000	C	-1.9099	-2.2940	0.0000	H	2.9640	2.8561	0.0000
C	2.1378	-0.9911	0.0000	C	-2.1701	-3.6460	0.0000	H	2.6478	-3.0815	0.0000
C	1.8294	-2.3432	0.0000	C	-1.1181	-4.5897	0.0000	H	-4.2255	3.1404	0.0000
C	-3.4113	2.4050	0.0000	C	0.1834	-4.1752	0.0000	H	1.6249	4.0668	0.0000
C	-2.0847	2.8413	0.0000	C	-2.6615	0.0835	0.0000	H	-0.2275	5.7195	0.0000
C	0.5837	3.7089	0.0000	C	-3.7120	1.0400	0.0000	H	-2.5962	4.9595	0.0000
C	-0.4747	4.6528	0.0000	C	-5.0694	0.5887	0.0000	H	-3.2145	-3.9948	0.0000
C	-1.7715	4.2378	0.0000	C	-5.3536	-0.7436	0.0000	H	-1.3646	-5.6566	0.0000
C	-1.0268	1.8922	0.0000	C	-4.3094	-1.7019	0.0000	H	1.0056	-4.8995	0.0000
C	-1.3226	0.5176	0.0000	C	-2.9920	-1.3135	0.0000	H	-5.8703	1.3369	0.0000
C	-0.2439	-0.4530	0.0000	C	3.7989	0.8342	0.0000	H	-6.3906	-1.0953	0.0000
C	1.0887	-0.0283	0.0000	C	3.5197	-0.5426	0.0000	H	-4.5577	-2.7746	0.0000
C	1.4175	1.3812	0.0000	C	4.5900	-1.4573	0.0000	H	4.3621	-2.5342	0.0000
C	0.3308	2.3590	0.0000	C	5.8951	-1.0113	0.0000	H	6.7218	-1.7291	0.0000
C	0.4944	-2.7842	0.0000	C	6.1704	0.3630	0.0000	H	7.2101	0.7064	0.0000
C	-0.5543	-1.8347	0.0000	C	5.1370	1.2760	0.0000	H	5.3469	2.3517	0.0000

Table 3.538: Table of thermodynamic data as a function of temperature for Benzo[*e*]phenanthro[1,10,9,8-*opqra*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.158	537.784	537.784	∞
100	119.395	367.236	856.469	-48.923	564.317	611.221	-319.263
200	245.048	486.632	641.534	-30.980	550.276	663.733	-173.346
250	316.876	548.979	616.753	-16.943	543.673	692.860	-144.762
298.15	386.720	610.778	610.778	0.000	537.784	722.143	-126.514
300	389.371	613.179	610.786	0.718	537.566	723.284	-125.932
350	459.105	678.490	615.784	21.947	532.131	754.680	-112.627
400	523.858	744.085	627.723	46.545	527.409	786.792	-102.742
450	582.591	809.239	644.279	74.232	523.312	819.466	-95.119
500	635.126	873.393	663.993	104.700	519.748	852.591	-89.068
600	723.187	997.296	709.309	172.792	513.912	919.738	-80.069
700	792.638	1114.198	758.887	248.718	509.598	987.744	-73.705
800	848.085	1223.794	810.226	330.854	506.638	1056.256	-68.965
900	893.033	1326.368	861.939	417.986	504.858	1125.059	-65.295
1000	929.971	1422.432	913.237	509.195	504.099	1194.019	-62.368
1100	960.668	1512.551	963.667	603.773	504.157	1263.025	-59.975
1200	986.415	1597.276	1012.973	701.163	504.891	1331.975	-57.978
1300	1008.179	1677.115	1061.020	800.923	506.115	1400.855	-56.286
1400	1026.703	1752.525	1107.745	902.691	507.691	1469.630	-54.831
1500	1042.568	1823.915	1153.131	1006.175	509.543	1538.287	-53.567
1600	1056.234	1891.648	1197.190	1111.132	511.532	1606.803	-52.456
1700	1068.069	1956.045	1239.950	1217.361	513.585	1675.166	-51.471
1800	1078.372	2017.392	1281.451	1324.695	515.623	1743.481	-50.593
1900	1087.384	2075.944	1321.737	1432.992	517.616	1811.623	-49.804
2000	1095.303	2131.925	1360.857	1542.135	519.511	1879.693	-49.092
2100	1102.293	2185.538	1398.860	1652.022	521.222	1947.656	-48.444
2200	1108.488	2236.962	1435.795	1762.567	522.751	2015.543	-47.854
2300	1114.000	2286.360	1471.709	1873.697	524.097	2083.367	-47.314
2400	1118.923	2333.878	1506.649	1985.348	525.180	2151.080	-46.816
2500	1123.335	2379.645	1540.660	2097.464	526.016	2218.883	-46.360
2600	1127.303	2423.782	1573.782	2210.000	526.568	2286.523	-45.936
2700	1130.883	2466.395	1606.057	2322.912	526.840	2354.235	-45.544
2800	1134.123	2507.582	1637.523	2436.165	526.805	2421.962	-45.181
2900	1137.063	2547.432	1668.216	2549.727	526.431	2489.637	-44.842
3000	1139.739	2586.026	1698.170	2663.569	525.769	2557.362	-44.527
3100	1142.180	2623.438	1727.417	2777.667	524.731	2625.023	-44.230
3200	1144.413	2659.737	1755.988	2891.998	523.366	2692.809	-43.955
3300	1146.461	2694.984	1783.911	3006.543	521.655	2760.691	-43.697
3400	1148.343	2729.238	1811.213	3121.284	519.564	2828.526	-43.454
3500	1150.076	2762.551	1837.920	3236.207	517.103	2896.407	-43.226
3600	1151.675	2794.972	1864.057	3351.295	514.295	2964.469	-43.012
3700	1153.153	2826.547	1889.645	3466.538	511.106	3032.629	-42.812
3800	1154.523	2857.318	1914.707	3581.922	507.506	3100.816	-42.623
3900	1155.795	2887.324	1939.263	3697.439	503.543	3169.036	-42.444
4000	1156.976	2916.601	1963.332	3813.078	499.198	3237.529	-42.277
4100	1158.077	2945.184	1986.932	3928.831	494.431	3306.048	-42.119
4200	1159.103	2973.103	2010.081	4044.691	489.275	3374.679	-41.969
4300	1160.062	3000.389	2032.796	4160.650	483.714	3443.332	-41.827
4400	1160.959	3027.068	2055.091	4276.701	477.757	3512.224	-41.695
4500	1161.799	3053.168	2076.981	4392.840	471.424	3581.320	-41.570
4600	1162.586	3078.712	2098.481	4509.059	464.651	3650.576	-41.453
4700	1163.326	3103.723	2119.604	4625.355	457.459	3719.849	-41.341
4800	1164.022	3128.222	2140.363	4741.723	449.899	3789.403	-41.236
4900	1164.677	3152.230	2160.769	4858.159	441.886	3858.960	-41.136
5000	1165.295	3175.766	2180.834	4974.657	433.529	3928.900	-41.044

3.539. Benzo[3,4]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-12-6
Point Group: C₁

Length: 14.30 Å
Width: 11.51 Å
Breadth: 5.053 Å
L/B Ratio: 1.242

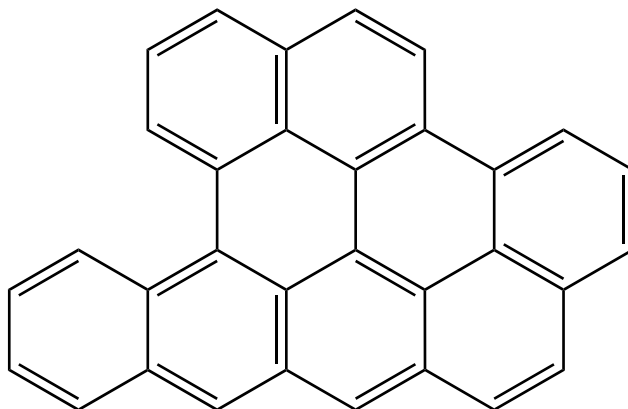
Cartesian coordinates:

C	1.7141	0.0960	0.0381	C	-5.0858	-1.5778	0.5486	H	-5.4831	0.5526	0.5772
C	1.3056	-1.2386	-0.1340	C	-4.1409	-2.5673	0.3722	H	-6.1306	-1.8410	0.7438
C	2.2879	-2.2825	-0.2837	C	0.7496	1.1401	0.1449	H	-4.4288	-3.6239	0.4141
C	3.6219	-1.9863	-0.2743	C	-0.6169	0.8512	-0.0235	H	-2.1383	-4.2963	-0.0532
C	4.0685	-0.6418	-0.0798	C	-3.0158	1.5202	0.0119	H	0.1693	-4.9889	-0.4553
C	3.1157	0.3875	0.0978	C	-1.6634	1.8615	-0.1898	H	2.5797	-4.4289	-0.5783
C	-0.0702	-1.5482	-0.1169	C	-1.3821	3.1690	-0.6243	H	4.3732	-2.7754	-0.4022
C	-0.4914	-2.9254	-0.1707	C	-2.3735	4.1263	-0.7417	H	-0.3514	3.4477	-0.8833
C	0.5155	-3.9528	-0.3624	C	-3.6953	3.8052	-0.4343	H	-2.1208	5.1378	-1.0763
C	1.8237	-3.6496	-0.4269	C	-4.0099	2.5086	-0.0756	H	-4.4772	4.5684	-0.4985
C	-1.0237	-0.5138	-0.0346	C	3.5613	1.7095	0.3371	H	-5.0544	2.2279	0.1307
C	-2.4089	-0.8697	0.0955	C	4.9253	1.9906	0.3685	H	6.1744	-1.1283	-0.1975
C	-2.7936	-2.2272	0.1442	C	5.8555	0.9713	0.1681	H	6.9252	1.2054	0.1884
C	-1.8108	-3.2494	-0.0335	C	5.4381	-0.3302	-0.0493	H	5.2670	3.0153	0.5534
C	-3.4005	0.1328	0.2207	C	1.2528	2.4533	0.4772	H	2.9205	3.7344	0.8298
C	-4.7195	-0.2323	0.4655	C	2.5717	2.7288	0.5673	H	0.5246	3.2508	0.6803

Table 3.539: Table of thermodynamic data as a function of temperature for Benzo[3,4]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.491	519.494	519.494	∞
100	115.775	356.857	843.031	-48.617	546.332	594.275	-310.411
200	243.711	474.406	629.042	-30.927	532.038	647.941	-169.221
250	316.403	536.554	604.290	-16.934	525.392	677.685	-141.592
298.15	386.755	598.318	598.318	0.000	519.494	707.567	-123.960
300	389.421	600.719	598.325	0.718	519.276	708.732	-123.399
350	459.441	666.061	603.326	21.957	513.851	740.750	-110.549
400	524.337	731.712	615.272	46.576	509.150	773.482	-101.004
450	583.128	796.926	631.840	74.289	505.079	806.774	-93.646
500	635.676	861.138	651.569	104.784	501.542	840.513	-87.806
600	723.702	985.138	696.922	172.930	495.760	908.880	-79.123
700	793.093	1102.116	746.538	248.904	491.494	978.098	-72.985
800	848.483	1211.768	797.914	331.083	488.577	1047.815	-68.414
900	893.381	1314.387	849.662	418.252	486.834	1117.818	-64.875
1000	930.277	1410.485	900.991	509.494	486.107	1187.974	-62.052
1100	960.938	1500.632	951.449	604.100	486.194	1258.174	-59.744
1200	986.655	1585.379	1000.781	701.517	486.954	1328.314	-57.819
1300	1008.394	1665.235	1048.852	801.299	488.201	1398.383	-56.187
1400	1026.896	1740.661	1095.598	903.088	489.797	1468.346	-54.784
1500	1042.742	1812.063	1141.004	1006.590	491.667	1538.188	-53.563
1600	1056.391	1879.807	1185.080	1111.563	493.673	1607.889	-52.491
1700	1068.212	1944.213	1227.856	1217.807	495.741	1677.436	-51.540
1800	1078.503	2005.569	1269.372	1325.155	497.792	1746.934	-50.694
1900	1087.504	2064.127	1309.672	1433.465	499.798	1816.258	-49.931
2000	1095.413	2120.114	1348.804	1542.619	501.705	1885.509	-49.243
2100	1102.394	2173.732	1386.819	1652.516	503.426	1954.653	-48.618
2200	1108.581	2225.161	1423.764	1763.071	504.965	2023.721	-48.048
2300	1114.087	2274.563	1459.689	1874.210	506.320	2092.725	-47.526
2400	1119.003	2322.084	1494.638	1985.869	507.411	2161.616	-47.045
2500	1123.410	2367.855	1528.657	2097.994	508.255	2230.599	-46.605
2600	1127.373	2411.994	1561.788	2210.536	508.814	2299.418	-46.195
2700	1130.948	2454.610	1594.071	2323.455	509.093	2368.309	-45.817
2800	1134.184	2495.799	1625.544	2436.715	509.064	2437.214	-45.466
2900	1137.120	2535.651	1656.243	2550.282	508.696	2506.068	-45.138
3000	1139.792	2574.247	1686.204	2664.130	508.039	2574.971	-44.833
3100	1142.231	2611.661	1715.457	2778.233	507.006	2643.809	-44.547
3200	1144.461	2647.961	1744.033	2892.569	505.647	2712.773	-44.281
3300	1146.506	2683.210	1771.962	3007.119	503.940	2781.833	-44.032
3400	1148.385	2717.465	1799.269	3121.865	501.854	2850.844	-43.797
3500	1150.116	2750.779	1825.981	3236.791	499.397	2919.903	-43.576
3600	1151.713	2783.201	1852.122	3351.883	496.593	2989.142	-43.370
3700	1153.190	2814.777	1877.715	3467.129	493.407	3058.479	-43.177
3800	1154.558	2845.549	1902.781	3582.518	489.811	3127.842	-42.994
3900	1155.828	2875.556	1927.341	3698.038	485.851	3197.240	-42.821
4000	1157.008	2904.834	1951.414	3813.680	481.510	3266.909	-42.661
4100	1158.107	2933.417	1975.018	3929.437	476.746	3336.605	-42.508
4200	1159.132	2961.337	1998.171	4045.299	471.593	3406.413	-42.364
4300	1160.089	2988.624	2020.889	4161.261	466.034	3476.242	-42.227
4400	1160.985	3015.304	2043.187	4277.315	460.081	3546.311	-42.099
4500	1161.824	3041.404	2065.081	4393.456	453.750	3616.583	-41.979
4600	1162.611	3066.948	2086.584	4509.678	446.980	3687.015	-41.867
4700	1163.349	3091.960	2107.709	4625.976	439.790	3757.465	-41.759
4800	1164.044	3116.460	2128.471	4742.346	432.232	3828.196	-41.658
4900	1164.698	3140.468	2148.880	4858.784	424.222	3898.928	-41.562
5000	1165.315	3164.004	2168.948	4975.285	415.867	3970.044	-41.474

3.540. Anthra[3,2,1,9-*pqra*]benzo[*cd*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-18-2
Point Group: C₁

Length: 15.27 Å
Width: 11.76 Å
Breadth: 4.906 Å
L/B Ratio: 1.298

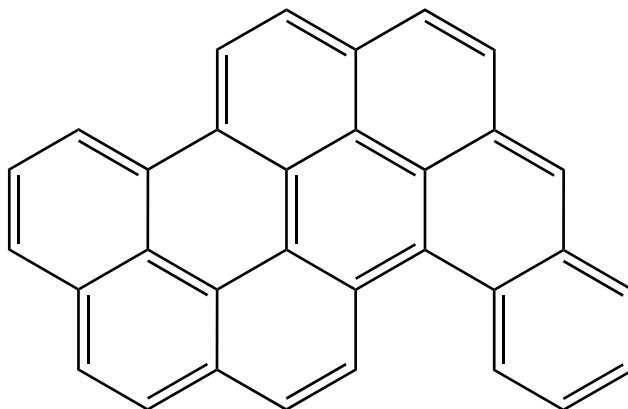
Cartesian coordinates:

C	5.5893	0.3529	-0.6892	C	-2.9487	0.6650	-0.0443	H	6.4528	-0.2366	-1.0151
C	5.7635	1.7392	-0.4335	C	-3.1718	-0.7181	-0.2021	H	6.7623	2.1777	-0.5254
C	4.6879	2.5007	-0.0986	C	-1.6148	1.1680	0.0966	H	4.7935	3.5773	0.0786
C	4.3685	-0.2320	-0.5413	C	-0.5259	0.2980	0.0798	H	4.2587	-1.3029	-0.7611
C	3.2156	0.5116	-0.1299	C	1.9330	-0.0620	0.0741	H	2.4281	3.8223	0.3871
C	3.3849	1.9168	0.0181	C	0.8164	0.8004	0.1465	H	0.0383	4.1539	0.4454
C	2.2829	2.7435	0.2479	C	1.6911	-1.5004	0.2100	H	-2.3809	4.5296	0.4205
C	0.9968	2.2088	0.2485	C	1.1926	-4.2849	0.3274	H	-4.6817	3.6393	0.1725
C	-0.1349	3.0764	0.3315	C	2.4450	-3.7865	0.5942	H	-6.1954	1.7527	-0.1787
C	-1.4077	2.5816	0.2450	C	2.6886	-2.4067	0.5413	H	-6.5758	-0.6808	-0.4824
C	-2.5615	3.4571	0.2834	C	0.1284	-3.3935	0.0756	H	-4.6550	-2.2652	-0.4880
C	-3.8110	2.9736	0.1491	C	0.3640	-2.0027	0.0625	H	1.0038	-5.3642	0.3320
C	-4.0520	1.5576	-0.0309	C	-0.7523	-1.1141	-0.0353	H	3.2683	-4.4641	0.8442
C	-5.3415	1.0658	-0.1873	C	-2.0459	-1.6182	-0.1771	H	3.7063	-2.0568	0.7625
C	-5.5549	-0.3054	-0.3562	C	-2.2419	-3.0293	-0.2619	H	-3.2675	-3.3984	-0.4162
C	-4.4908	-1.1841	-0.3615	C	-1.1959	-3.8878	-0.1322	H	-1.3496	-4.9721	-0.1736

Table 3.540: Table of thermodynamic data as a function of temperature for Anthra[3,2,1,9-*ppra*]benzo[*cd*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.619	524.900	524.900	∞
100	116.534	357.478	844.569	-48.709	551.647	599.527	-313.154
200	244.125	475.464	630.255	-30.958	537.414	653.105	-170.570
250	316.706	537.691	605.481	-16.947	530.784	682.794	-142.659
298.15	387.010	599.504	599.504	0.000	524.900	712.620	-124.845
300	389.674	601.906	599.511	0.718	524.682	713.782	-124.278
350	459.672	667.286	604.515	21.970	519.270	745.740	-111.293
400	524.556	732.967	616.467	46.600	514.580	778.410	-101.648
450	583.338	798.206	633.043	74.323	510.519	811.638	-94.211
500	635.877	862.440	652.781	104.829	506.993	845.313	-88.307
600	723.880	986.475	698.152	172.994	501.230	913.548	-79.530
700	793.246	1103.478	747.785	248.985	496.980	982.631	-73.323
800	848.612	1213.149	799.177	331.178	494.078	1052.211	-68.701
900	893.488	1315.781	850.939	418.358	492.346	1122.075	-65.122
1000	930.365	1411.890	902.280	509.610	491.629	1192.091	-62.267
1100	961.012	1502.044	952.749	604.224	491.724	1262.151	-59.933
1200	986.716	1586.797	1002.091	701.647	492.491	1332.149	-57.986
1300	1008.445	1666.658	1050.170	801.435	493.743	1402.076	-56.335
1400	1026.939	1742.087	1096.924	903.229	495.345	1471.896	-54.916
1500	1042.778	1813.492	1142.336	1006.735	497.218	1541.596	-53.682
1600	1056.422	1881.238	1186.419	1111.711	499.227	1611.153	-52.598
1700	1068.239	1945.646	1229.200	1217.958	501.298	1680.557	-51.636
1800	1078.526	2007.003	1270.721	1325.308	503.352	1749.911	-50.780
1900	1087.524	2065.562	1311.025	1433.621	505.360	1819.092	-50.009
2000	1095.431	2121.550	1350.162	1542.777	507.268	1888.200	-49.314
2100	1102.410	2175.169	1388.180	1652.676	508.992	1957.200	-48.682
2200	1108.595	2226.599	1425.129	1763.232	510.532	2026.124	-48.105
2300	1114.099	2276.001	1461.057	1874.372	511.888	2094.984	-47.578
2400	1119.014	2323.523	1496.009	1986.032	512.980	2163.732	-47.091
2500	1123.420	2369.294	1530.031	2098.158	513.826	2232.570	-46.646
2600	1127.382	2413.434	1563.164	2210.702	514.385	2301.246	-46.232
2700	1130.956	2456.050	1595.449	2323.621	514.665	2369.992	-45.849
2800	1134.191	2497.240	1626.925	2436.882	514.637	2438.754	-45.495
2900	1137.127	2537.092	1657.626	2550.450	514.270	2507.463	-45.163
3000	1139.799	2575.688	1687.589	2664.298	513.614	2576.222	-44.855
3100	1142.236	2613.102	1716.844	2778.402	512.581	2644.916	-44.566
3200	1144.466	2649.402	1745.422	2892.738	511.222	2713.736	-44.296
3300	1146.511	2684.651	1773.352	3007.289	509.517	2782.651	-44.045
3400	1148.390	2718.906	1800.661	3122.035	507.431	2851.519	-43.807
3500	1150.120	2752.221	1827.374	3236.962	504.974	2920.433	-43.584
3600	1151.717	2784.643	1853.517	3352.055	502.171	2989.529	-43.376
3700	1153.194	2816.219	1879.111	3467.301	498.985	3058.721	-43.181
3800	1154.562	2846.991	1904.178	3582.690	495.390	3127.940	-42.996
3900	1155.831	2876.998	1928.739	3698.210	491.430	3197.194	-42.821
4000	1157.011	2906.277	1952.813	3813.853	487.089	3266.719	-42.658
4100	1158.110	2934.860	1976.418	3929.610	482.326	3336.271	-42.504
4200	1159.135	2962.780	1999.572	4045.473	477.172	3405.934	-42.358
4300	1160.092	2990.066	2022.291	4161.434	471.614	3475.619	-42.220
4400	1160.987	3016.747	2044.590	4277.489	465.661	3545.544	-42.090
4500	1161.826	3042.847	2066.485	4393.630	459.330	3615.671	-41.969
4600	1162.613	3068.391	2087.988	4509.852	452.560	3685.959	-41.855
4700	1163.352	3093.403	2109.115	4626.151	445.371	3756.264	-41.745
4800	1164.046	3117.902	2129.877	4742.521	437.813	3826.851	-41.644
4900	1164.700	3141.911	2150.287	4858.959	429.803	3897.439	-41.546
5000	1165.317	3165.447	2170.355	4975.460	421.448	3968.411	-41.457

3.541. Dibenzo[*a,ghi*]naphtho[8,1,2-*klm*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-03-5
Point Group: C₁

Length: 15.48 Å
Width: 11.57 Å
Breadth: 5.016 Å
L/B Ratio: 1.338

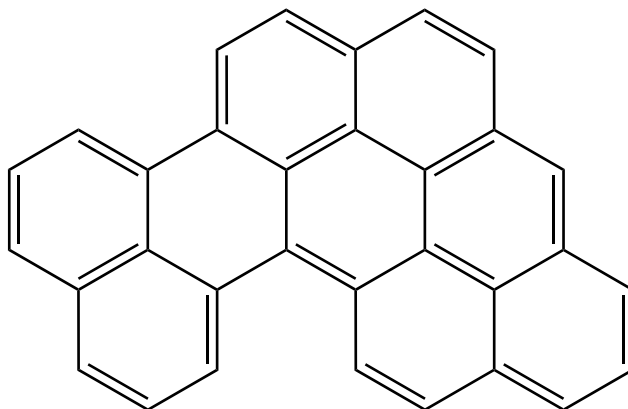
Cartesian coordinates:

C	-4.2637	2.6750	-0.1323	C	-1.9640	-3.0676	0.1703	H	1.4996	3.0016	-0.7445
C	-4.3206	1.2537	0.0716	C	1.7525	-1.0501	-0.1433	H	-0.6011	4.2604	-0.8372
C	-3.1262	0.5034	0.0529	C	2.9397	-1.8387	-0.2405	H	-2.9332	-3.5764	0.2897
C	-1.8692	1.1711	-0.1348	C	2.8427	-3.2775	-0.3298	H	-0.8319	-4.8929	0.0480
C	-1.8510	2.5572	-0.3557	C	1.6509	-3.9026	-0.2491	H	1.5765	-4.9951	-0.2967
C	-3.0803	3.2982	-0.3484	C	1.8244	0.3504	-0.0739	H	3.7723	-3.8460	-0.4501
C	-3.1781	-0.9019	0.2135	C	3.1100	0.9505	0.1349	H	5.0887	-1.8203	-0.3749
C	-4.4090	-1.5196	0.4147	C	4.2763	0.1611	-0.0139	H	6.4501	0.1260	-0.0599
C	-5.5848	-0.7692	0.4541	C	4.1750	-1.2276	-0.2414	H	6.6876	2.5246	0.5642
C	-5.5476	0.6017	0.2802	C	0.5825	1.1016	-0.2137	H	4.6598	3.8752	1.0486
C	-0.6518	0.4383	-0.0988	C	-0.6165	3.1908	-0.5974	H	2.4183	2.9180	0.7811
C	-0.7121	-0.9957	0.0052	C	0.5566	2.4787	-0.5336	H	-6.4731	1.1880	0.3018
C	-1.9422	-1.6658	0.1392	C	5.5669	0.7516	0.1138	H	-6.5418	-1.2754	0.6189
C	0.4874	-1.7362	-0.0899	C	5.6994	2.0650	0.4618	H	-4.4429	-2.6133	0.5363
C	0.4341	-3.1445	-0.0981	C	4.5435	2.8382	0.7163	H	-3.0336	4.3801	-0.5176
C	-0.7983	-3.7973	0.0413	C	3.2976	2.2984	0.5580	H	-5.2037	3.2384	-0.1145

Table 3.541: Table of thermodynamic data as a function of temperature for Dibenz[*a,ghi*]naphtho[8,1,2-*klm*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-55.418	497.354	497.354	∞
100	115.722	357.412	842.669	-48.526	524.284	572.171	-298.865
200	243.192	474.745	629.092	-30.869	509.957	625.792	-163.437
250	315.802	536.768	604.385	-16.904	503.282	655.522	-136.961
298.15	386.128	598.423	598.423	0.000	497.354	685.396	-120.076
300	388.793	600.820	598.430	0.717	497.135	686.561	-119.538
350	458.826	666.066	603.423	21.925	491.679	718.576	-107.239
400	523.756	731.637	615.353	46.514	486.948	751.310	-98.109
450	582.593	796.785	631.899	74.199	482.848	784.607	-91.073
500	635.190	860.944	651.606	104.669	479.287	818.355	-85.491
600	723.307	984.863	696.913	172.770	473.460	886.745	-77.196
700	792.774	1101.786	746.487	248.709	469.159	955.994	-71.336
800	848.223	1211.400	797.826	330.859	466.213	1025.746	-66.973
900	893.167	1313.990	849.541	418.004	464.446	1095.787	-63.597
1000	930.097	1410.068	900.841	509.226	463.700	1165.984	-60.904
1100	960.787	1500.199	951.275	603.816	463.770	1236.227	-58.702
1200	986.526	1584.933	1000.584	701.219	464.517	1306.411	-56.865
1300	1008.282	1664.781	1048.635	800.989	465.751	1376.525	-55.308
1400	1026.799	1740.198	1095.364	902.767	467.337	1446.534	-53.970
1500	1042.657	1811.594	1140.754	1006.260	469.198	1516.422	-52.805
1600	1056.316	1879.333	1184.817	1111.226	471.195	1586.170	-51.782
1700	1068.145	1943.735	1227.580	1217.463	473.256	1655.765	-50.874
1800	1078.443	2005.087	1269.085	1324.804	475.302	1725.310	-50.066
1900	1087.450	2063.642	1309.374	1433.108	477.302	1794.683	-49.338
2000	1095.364	2119.626	1348.497	1542.257	479.203	1863.983	-48.681
2100	1102.350	2173.242	1386.503	1652.150	480.920	1933.176	-48.084
2200	1108.541	2224.669	1423.441	1762.701	482.455	2002.292	-47.539
2300	1114.049	2274.069	1459.358	1873.835	483.805	2071.346	-47.041
2400	1118.969	2321.588	1494.301	1985.491	484.893	2140.287	-46.581
2500	1123.378	2367.358	1528.313	2097.612	485.734	2209.319	-46.160
2600	1127.343	2411.496	1561.438	2210.152	486.290	2278.188	-45.768
2700	1130.921	2454.111	1593.715	2323.068	486.566	2347.128	-45.407
2800	1134.158	2495.299	1625.183	2436.325	486.534	2416.084	-45.072
2900	1137.096	2535.150	1655.878	2549.890	486.164	2484.987	-44.759
3000	1139.770	2573.746	1685.834	2663.735	485.505	2553.940	-44.467
3100	1142.210	2611.159	1715.083	2777.836	484.470	2622.829	-44.193
3200	1144.442	2647.458	1743.655	2892.170	483.108	2691.843	-43.939
3300	1146.488	2682.706	1771.580	3006.718	481.400	2760.953	-43.701
3400	1148.368	2716.961	1798.884	3121.462	479.312	2830.015	-43.477
3500	1150.100	2750.274	1825.592	3236.387	476.853	2899.124	-43.266
3600	1151.698	2782.696	1851.730	3351.478	474.047	2968.414	-43.070
3700	1153.175	2814.272	1877.320	3466.722	470.860	3037.801	-42.885
3800	1154.544	2845.044	1902.383	3582.109	467.263	3107.215	-42.711
3900	1155.814	2875.050	1926.940	3697.628	463.302	3176.664	-42.546
4000	1156.995	2904.328	1951.011	3813.269	458.959	3246.383	-42.393
4100	1158.095	2932.911	1974.612	3929.024	454.194	3316.130	-42.247
4200	1159.121	2960.831	1997.763	4044.886	449.039	3385.988	-42.110
4300	1160.078	2988.117	2020.478	4160.846	443.480	3455.868	-41.980
4400	1160.975	3014.797	2042.774	4276.899	437.525	3525.988	-41.858
4500	1161.814	3040.897	2064.666	4393.039	431.193	3596.311	-41.744
4600	1162.601	3066.441	2086.167	4509.260	424.422	3666.794	-41.637
4700	1163.340	3091.452	2107.291	4625.558	417.231	3737.294	-41.535
4800	1164.036	3115.951	2128.050	4741.927	409.673	3808.075	-41.439
4900	1164.690	3139.960	2148.457	4858.363	401.661	3878.859	-41.348
5000	1165.307	3163.496	2168.523	4974.864	393.305	3950.026	-41.265

3.542. Dibenzo[*ghi,lm*]naphtho[1,8-*ab*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120864-23-5
Point Group: C₁

Length: 15.41 Å
Width: 11.48 Å
Breadth: 5.130 Å
L/B Ratio: 1.342

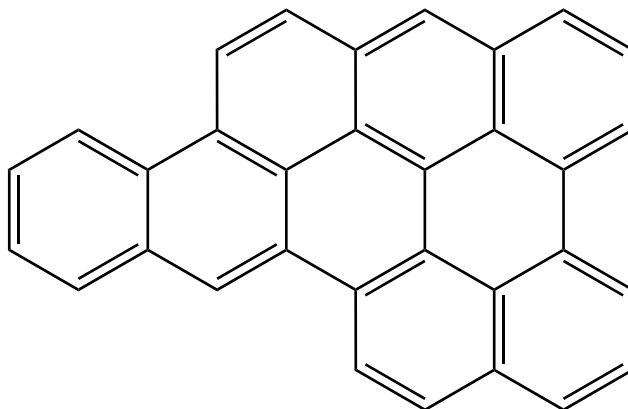
Cartesian coordinates:

C	4.4953	-1.2907	-0.5347	C	-2.6289	-3.4245	0.3168	H	3.1628	-3.4022	-0.2192
C	3.2677	-0.7339	-0.2355	C	-1.4024	-3.9809	0.2713	H	1.1504	-4.8370	0.0638
C	3.1622	0.6649	0.0072	C	-1.7671	0.2225	-0.0494	H	-1.2704	-5.0670	0.3403
C	4.3440	1.4360	0.0503	C	-3.0747	0.7942	-0.1034	H	-3.5275	-4.0423	0.4279
C	5.5887	0.8392	-0.2794	C	-4.2173	-0.0259	0.0346	H	-4.9530	-2.0574	0.2873
C	5.6554	-0.4951	-0.5833	C	-4.0585	-1.4298	0.1909	H	-2.1982	4.0618	-0.7093
C	1.8944	1.2821	0.2547	C	-0.5983	1.0586	-0.1152	H	0.0482	3.1032	-0.5612
C	0.6676	0.5029	0.0527	C	-3.2436	2.1914	-0.2962	H	-6.3838	-0.0762	0.1227
C	0.8033	-0.9291	0.0264	C	-2.0617	2.9980	-0.4820	H	-6.6394	2.3735	-0.1860
C	2.0700	-1.5541	-0.1018	C	-0.8285	2.4612	-0.3952	H	-4.6441	3.8195	-0.4738
C	-0.3438	-1.7533	0.0899	C	-4.5154	2.7415	-0.3248	H	0.9501	3.0688	1.0109
C	-0.2156	-3.1673	0.1335	C	-5.6418	1.9221	-0.1665	H	3.0200	4.3684	1.1835
C	1.0421	-3.7468	0.0384	C	-5.5014	0.5633	0.0064	H	5.2023	3.3858	0.4915
C	2.1698	-2.9406	-0.1019	C	4.2800	2.7954	0.4555	H	6.4912	1.4608	-0.2801
C	-1.6400	-1.1639	0.0943	C	3.0790	3.3360	0.8229	H	6.6111	-0.9603	-0.8460
C	-2.8053	-1.9923	0.2063	C	1.8916	2.5816	0.7223	H	4.5670	-2.3743	-0.7145

Table 3.542: Table of thermodynamic data as a function of temperature for Dibenz[*ghi,lm*]naphtho[1,8-*ab*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.324	532.752	532.752	∞
100	115.066	355.740	840.784	-48.504	559.703	607.757	-317.453
200	243.144	472.801	627.220	-30.884	545.340	661.564	-172.779
250	315.969	534.839	602.500	-16.915	538.669	691.391	-144.455
298.15	386.401	596.534	596.534	0.000	532.752	721.357	-126.376
300	389.068	598.932	596.541	0.717	532.533	722.526	-125.800
350	459.140	664.224	601.537	21.940	527.092	754.634	-112.621
400	524.075	729.838	613.475	46.545	522.377	787.459	-102.830
450	582.899	795.023	630.032	74.246	518.293	820.845	-95.279
500	635.477	859.212	649.751	104.731	514.746	854.680	-89.286
600	723.555	983.181	695.083	172.859	508.947	923.241	-80.374
700	792.988	1100.139	744.681	248.821	504.668	992.656	-74.071
800	848.410	1209.780	796.041	330.991	501.743	1062.572	-69.377
900	893.332	1312.391	847.776	418.154	499.993	1132.774	-65.743
1000	930.245	1408.485	899.094	509.391	499.263	1203.130	-62.844
1100	960.919	1498.629	949.543	603.995	499.347	1273.530	-60.474
1200	986.645	1583.375	998.866	701.410	500.106	1343.870	-58.496
1300	1008.390	1663.231	1046.930	801.192	501.352	1414.140	-56.820
1400	1026.897	1738.656	1093.670	902.980	502.948	1484.303	-55.379
1500	1042.746	1810.059	1139.071	1006.483	504.818	1554.346	-54.126
1600	1056.398	1877.803	1183.143	1111.456	506.824	1624.247	-53.025
1700	1068.220	1942.210	1225.915	1217.701	508.893	1693.994	-52.049
1800	1078.512	2003.566	1267.427	1325.050	510.945	1763.692	-51.180
1900	1087.513	2062.124	1307.724	1433.361	512.952	1833.216	-50.398
2000	1095.423	2118.112	1346.854	1542.516	514.860	1902.668	-49.692
2100	1102.404	2171.730	1384.866	1652.414	516.582	1972.012	-49.050
2200	1108.591	2223.160	1421.809	1762.970	518.122	2041.280	-48.465
2300	1114.096	2272.562	1457.732	1874.110	519.478	2110.484	-47.930
2400	1119.013	2320.084	1492.679	1985.770	520.570	2179.576	-47.436
2500	1123.419	2365.855	1526.697	2097.895	521.415	2248.758	-46.984
2600	1127.382	2409.995	1559.826	2210.439	521.975	2317.777	-46.564
2700	1130.957	2452.611	1592.107	2323.359	522.255	2386.868	-46.176
2800	1134.192	2493.800	1623.579	2436.619	522.227	2455.973	-45.816
2900	1137.128	2533.653	1654.278	2550.187	521.859	2525.027	-45.480
3000	1139.800	2572.249	1684.237	2664.036	521.203	2594.129	-45.167
3100	1142.238	2609.663	1713.489	2778.139	520.171	2663.167	-44.873
3200	1144.468	2645.963	1742.064	2892.476	518.812	2732.332	-44.600
3300	1146.513	2681.212	1769.992	3007.027	517.107	2801.591	-44.345
3400	1148.392	2715.467	1797.299	3121.773	515.021	2870.802	-44.104
3500	1150.122	2748.782	1824.010	3236.700	512.564	2940.061	-43.877
3600	1151.719	2781.204	1850.150	3351.793	509.761	3009.500	-43.666
3700	1153.196	2812.781	1875.743	3467.040	506.576	3079.036	-43.467
3800	1154.563	2843.553	1900.808	3582.429	502.981	3148.599	-43.280
3900	1155.833	2873.560	1925.367	3697.949	499.021	3218.197	-43.102
4000	1157.013	2902.838	1949.440	3813.592	494.680	3288.065	-42.937
4100	1158.112	2931.421	1973.043	3929.349	489.917	3357.961	-42.780
4200	1159.137	2959.341	1996.195	4045.212	484.764	3427.968	-42.632
4300	1160.094	2986.628	2018.913	4161.174	479.206	3497.997	-42.491
4400	1160.989	3013.308	2041.210	4277.229	473.253	3568.266	-42.360
4500	1161.828	3039.408	2063.104	4393.370	466.922	3638.737	-42.236
4600	1162.615	3064.953	2084.606	4509.593	460.153	3709.369	-42.120
4700	1163.353	3089.964	2105.732	4625.892	452.963	3780.018	-42.009
4800	1164.048	3114.464	2126.493	4742.262	445.406	3850.948	-41.906
4900	1164.702	3138.473	2146.901	4858.700	437.396	3921.881	-41.807
5000	1165.319	3162.009	2166.969	4975.201	429.041	3993.196	-41.716

3.543. Dibenzo[*cd,k*]naphtho[3,2,1,8-*pqra*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-02-4
Point Group: C_s

Length: 16.11 Å
Width: 11.96 Å
Breadth: 3.886 Å
L/B Ratio: 1.347

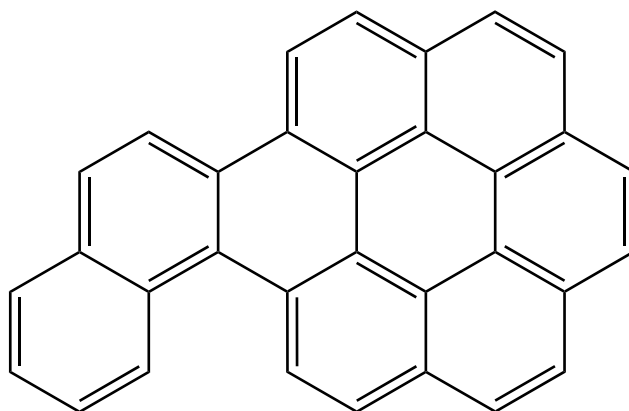
Cartesian coordinates:

C	6.3932	-0.1217	0.0000	C	0.3228	-1.2019	0.0000	H	7.3830	-0.5898	0.0000
C	6.2994	1.2906	0.0000	C	0.4023	-2.6253	0.0000	H	7.2186	1.8854	0.0000
C	5.0756	1.8997	0.0000	C	1.7022	-3.2469	0.0000	H	4.9929	2.9925	0.0000
C	5.2620	-0.8892	0.0000	C	2.8282	-2.4998	0.0000	H	5.3199	-1.9883	0.0000
C	3.9732	-0.2864	0.0000	C	2.7756	-1.0611	0.0000	H	2.5575	2.8479	0.0000
C	3.8827	1.1222	0.0000	C	1.5300	-0.4225	0.0000	H	-5.5252	-1.0465	0.0000
C	2.6155	1.7473	0.0000	C	-3.4923	0.7206	0.0000	H	-5.3564	-3.5273	0.0000
C	1.4516	1.0048	0.0000	C	-3.6522	3.5266	0.0000	H	-3.1307	-4.6372	0.0000
C	-3.4033	-0.7369	0.0000	C	-4.7956	2.7666	0.0000	H	-0.6932	-4.4808	0.0000
C	-4.5336	-1.5251	0.0000	C	-4.7168	1.3635	0.0000	H	1.7506	-4.3419	0.0000
C	-4.4365	-2.9332	0.0000	C	-2.3825	2.9006	0.0000	H	3.8244	-2.9686	0.0000
C	-3.2133	-3.5444	0.0000	C	-2.2962	1.4936	0.0000	H	-3.7069	4.6210	0.0000
C	-2.1134	-1.3542	0.0000	C	-1.0112	0.8665	0.0000	H	-5.7803	3.2456	0.0000
C	-2.0213	-2.7662	0.0000	C	0.1443	1.6406	0.0000	H	-5.6389	0.7618	0.0000
C	-0.7544	-3.3855	0.0000	C	0.0328	3.0603	0.0000	H	0.9615	3.6517	0.0000
C	-0.9289	-0.5756	0.0000	C	-1.1848	3.6725	0.0000	H	-1.2626	4.7657	0.0000

Table 3.543: Table of thermodynamic data as a function of temperature for Dibenzoc[cd,k]naphtho[3,2,1,8-pqra]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.853	495.579	495.579	∞
100	118.143	364.365	851.488	-48.712	522.323	569.515	-297.478
200	243.988	482.875	637.354	-30.896	508.156	622.365	-162.542
250	316.033	545.011	612.635	-16.906	501.505	651.685	-136.159
298.15	385.993	606.673	606.673	0.000	495.579	681.162	-119.334
300	388.647	609.069	606.681	0.717	495.360	682.311	-118.798
350	458.436	674.273	611.671	21.911	489.890	713.915	-106.544
400	523.216	739.781	623.591	46.476	485.135	746.241	-97.447
450	581.968	804.861	640.124	74.132	481.007	779.132	-90.437
500	634.523	868.950	659.812	104.569	477.413	812.477	-84.877
600	722.629	992.747	705.075	172.603	471.518	880.074	-76.616
700	792.130	1109.567	754.602	248.475	467.151	948.539	-70.779
800	847.628	1219.098	805.893	330.564	464.143	1017.518	-66.436
900	892.623	1321.621	857.563	417.652	462.319	1086.792	-63.074
1000	929.603	1417.644	908.822	508.822	461.521	1156.229	-60.394
1100	960.337	1507.730	959.216	603.365	461.544	1225.717	-58.203
1200	986.117	1592.427	1008.491	700.724	462.248	1295.149	-56.375
1300	1007.910	1672.243	1056.508	800.455	463.443	1364.515	-54.826
1400	1026.459	1747.634	1103.207	902.198	464.994	1433.779	-53.494
1500	1042.347	1819.008	1148.569	1005.659	466.822	1502.926	-52.335
1600	1056.032	1886.728	1192.606	1110.594	468.790	1571.933	-51.317
1700	1067.885	1951.113	1235.346	1216.804	470.824	1640.789	-50.414
1800	1078.203	2012.451	1276.828	1324.120	472.844	1709.597	-49.610
1900	1087.229	2070.993	1317.098	1432.402	474.821	1778.234	-48.886
2000	1095.161	2126.967	1356.202	1541.530	476.701	1846.800	-48.232
2100	1102.162	2180.573	1394.190	1651.403	478.398	1915.259	-47.638
2200	1108.366	2231.991	1431.112	1761.935	479.915	1983.643	-47.097
2300	1113.887	2281.384	1467.013	1873.053	481.249	2051.964	-46.601
2400	1118.818	2328.897	1501.942	1984.693	482.321	2120.174	-46.143
2500	1123.237	2374.661	1535.941	2096.800	483.147	2188.476	-45.725
2600	1127.212	2418.794	1569.053	2209.326	483.689	2256.615	-45.335
2700	1130.797	2461.403	1601.318	2322.229	483.953	2324.825	-44.976
2800	1134.042	2502.587	1632.775	2435.474	483.909	2393.052	-44.642
2900	1136.987	2542.435	1663.459	2549.028	483.527	2461.227	-44.331
3000	1139.668	2581.026	1693.405	2662.863	482.858	2529.452	-44.041
3100	1142.113	2618.436	1722.645	2776.953	481.813	2597.612	-43.769
3200	1144.350	2654.732	1751.208	2891.278	480.442	2665.899	-43.515
3300	1146.401	2689.978	1779.124	3005.817	478.725	2734.282	-43.279
3400	1148.286	2724.230	1806.420	3120.553	476.628	2802.617	-43.056
3500	1150.022	2757.541	1833.121	3235.470	474.161	2870.999	-42.846
3600	1151.624	2789.961	1859.252	3350.553	471.348	2939.562	-42.651
3700	1153.105	2821.535	1884.835	3465.790	468.154	3008.223	-42.468
3800	1154.478	2852.305	1909.891	3581.170	464.550	3076.911	-42.294
3900	1155.751	2882.309	1934.442	3696.683	460.582	3145.633	-42.130
4000	1156.935	2911.586	1958.506	3812.318	456.233	3214.627	-41.978
4100	1158.037	2940.167	1982.102	3928.067	451.462	3283.648	-41.833
4200	1159.065	2968.085	2005.247	4043.923	446.302	3352.781	-41.697
4300	1160.026	2995.370	2027.957	4159.878	440.737	3421.935	-41.567
4400	1160.924	3022.049	2050.248	4275.926	434.777	3491.330	-41.447
4500	1161.765	3048.148	2072.134	4392.061	428.440	3560.927	-41.333
4600	1162.555	3073.691	2093.631	4508.277	421.664	3630.685	-41.227
4700	1163.296	3098.701	2114.750	4624.570	414.469	3700.461	-41.125
4800	1163.993	3123.200	2135.505	4740.935	406.906	3770.517	-41.031
4900	1164.649	3147.207	2155.908	4857.367	398.890	3840.576	-40.940
5000	1165.267	3170.743	2175.970	4973.863	390.531	3911.018	-40.857

3.544. Naphtho[1,2-*a*]coronene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-90-7
Point Group: C₁

Length: 15.91 Å
Width: 11.65 Å
Breadth: 4.972 Å
L/B Ratio: 1.365

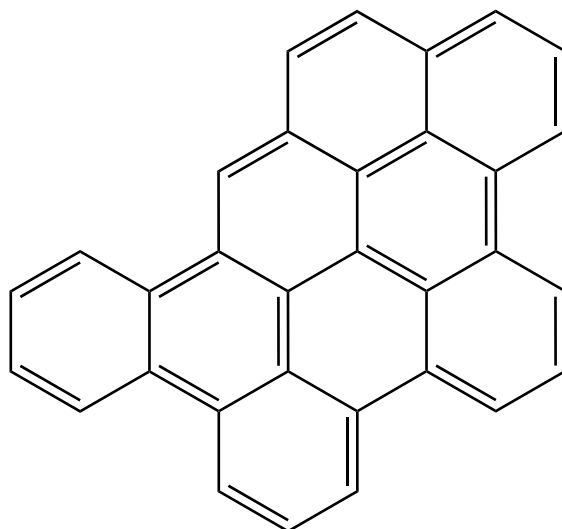
Cartesian coordinates:

C	1.3733	-2.2888	0.4379	C	-2.9163	0.3932	-0.1093	H	2.4005	-2.6370	0.6133
C	0.3562	-3.2011	0.4734	C	-4.2459	0.8160	-0.2405	H	0.5658	-4.2608	0.6595
C	-0.9868	-2.7924	0.2769	C	-5.2833	-0.1567	-0.2936	H	-4.1668	-4.0490	0.0499
C	-1.2580	-1.4249	0.1282	C	-4.9965	-1.4889	-0.1982	H	-1.8178	-4.8003	0.3540
C	-3.3452	-3.3243	0.0815	C	-3.6541	-1.9368	-0.0464	H	0.9900	3.9894	0.2597
C	-2.0573	-3.7362	0.2461	C	-2.6152	-0.9964	-0.0138	H	-1.3595	4.7347	0.0158
C	-0.1908	-0.4757	0.1226	C	1.8907	1.4238	0.2271	H	-3.7463	4.2051	-0.2615
C	1.1437	-0.9050	0.1967	C	2.2145	0.0674	0.1021	H	-5.5735	2.5301	-0.4165
C	-0.5041	0.9230	0.0690	C	4.2316	2.0392	0.4179	H	-6.3184	0.1850	-0.4079
C	0.5194	1.8690	0.1671	C	2.9230	2.3945	0.4174	H	-5.7978	-2.2359	-0.2345
C	0.1801	3.2508	0.1619	C	4.6019	0.6973	0.1037	H	5.0192	2.7752	0.6156
C	-1.1151	3.6664	0.0314	C	3.6049	-0.2772	-0.1145	H	2.6293	3.4423	0.5817
C	-1.8598	1.3525	-0.0449	C	4.0328	-1.5317	-0.6181	H	3.2848	-2.2881	-0.8916
C	-2.1676	2.7205	-0.0817	C	5.3630	-1.8229	-0.7939	H	5.6651	-2.7982	-1.1898
C	-3.5274	3.1318	-0.2225	C	6.3499	-0.8723	-0.4765	H	7.4077	-1.1284	-0.5936
C	-4.5302	2.2131	-0.3054	C	5.9723	0.3736	-0.0451	H	6.7251	1.1394	0.1749

Table 3.544: Table of thermodynamic data as a function of temperature for Naphtho[1,2-*a*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-55.245	474.779	474.779	∞
100	115.097	357.736	841.298	-48.356	501.879	549.733	-287.145
200	242.296	474.478	628.410	-30.786	487.465	603.353	-157.576
250	314.962	536.307	603.766	-16.865	480.746	633.102	-132.277
298.15	385.327	597.818	597.818	0.000	474.779	663.002	-116.153
300	387.993	600.209	597.825	0.715	474.559	664.168	-115.639
350	458.058	665.335	602.808	21.884	469.064	696.217	-103.903
400	523.023	730.805	614.717	46.435	464.295	728.990	-95.194
450	581.900	795.869	631.237	74.085	460.160	762.331	-88.487
500	634.541	859.957	650.914	104.521	456.565	796.126	-83.169
600	722.747	983.766	696.162	172.562	450.678	864.621	-75.270
700	792.297	1100.609	745.681	248.449	446.325	933.983	-69.693
800	847.816	1210.164	796.969	330.555	443.335	1003.856	-65.544
900	892.819	1312.710	848.640	417.663	441.530	1074.024	-62.333
1000	929.797	1408.753	899.901	508.853	440.752	1144.350	-59.774
1100	960.526	1498.857	950.299	603.415	440.794	1214.726	-57.681
1200	986.298	1583.571	999.577	700.793	441.516	1285.045	-55.935
1300	1008.081	1663.401	1047.600	800.542	442.729	1355.296	-54.455
1400	1026.621	1738.805	1094.304	902.301	444.296	1425.443	-53.183
1500	1042.498	1810.189	1139.671	1005.777	446.140	1495.472	-52.076
1600	1056.173	1877.918	1183.713	1110.727	448.123	1565.361	-51.103
1700	1068.017	1942.312	1226.459	1216.951	450.170	1635.097	-50.239
1800	1078.326	2003.657	1267.946	1324.280	452.203	1704.786	-49.471
1900	1087.344	2062.206	1308.220	1432.573	454.192	1774.302	-48.778
2000	1095.268	2118.185	1347.329	1541.712	456.083	1843.746	-48.153
2100	1102.261	2171.796	1385.322	1651.596	457.791	1913.083	-47.584
2200	1108.460	2223.219	1422.247	1762.138	459.317	1982.344	-47.066
2300	1113.974	2272.616	1458.153	1873.265	460.660	2051.542	-46.591
2400	1118.900	2320.132	1493.085	1984.913	461.740	2120.629	-46.153
2500	1123.314	2365.899	1527.088	2097.028	462.575	2189.807	-45.753
2600	1127.284	2410.035	1560.204	2209.561	463.124	2258.822	-45.379
2700	1130.865	2452.647	1592.473	2322.471	463.395	2327.909	-45.035
2800	1134.106	2493.834	1623.933	2435.723	463.358	2397.011	-44.716
2900	1137.048	2533.683	1654.620	2549.283	462.982	2466.061	-44.418
3000	1139.725	2572.277	1684.569	2663.123	462.319	2535.161	-44.140
3100	1142.167	2609.689	1713.811	2777.220	461.279	2604.196	-43.879
3200	1144.401	2645.987	1742.377	2891.550	459.913	2673.358	-43.637
3300	1146.450	2681.234	1770.296	3006.094	458.201	2742.614	-43.411
3400	1148.332	2715.487	1797.594	3120.834	456.110	2811.824	-43.198
3500	1150.066	2748.799	1824.298	3235.755	453.647	2881.080	-42.997
3600	1151.665	2781.221	1850.431	3350.843	450.838	2950.518	-42.810
3700	1153.145	2812.795	1876.016	3466.084	447.648	3020.053	-42.635
3800	1154.515	2843.566	1901.075	3581.468	444.048	3089.614	-42.469
3900	1155.787	2873.572	1925.627	3696.984	440.083	3159.210	-42.312
4000	1156.969	2902.849	1949.693	3812.623	435.738	3229.078	-42.167
4100	1158.070	2931.431	1973.291	3928.375	430.971	3298.973	-42.029
4200	1159.097	2959.350	1996.438	4044.234	425.813	3368.978	-41.899
4300	1160.056	2986.636	2019.149	4160.192	420.252	3439.007	-41.775
4400	1160.953	3013.315	2041.442	4276.243	414.294	3509.275	-41.660
4500	1161.793	3039.415	2063.330	4392.381	407.960	3579.745	-41.552
4600	1162.581	3064.959	2084.828	4508.600	401.187	3650.377	-41.450
4700	1163.321	3089.969	2105.949	4624.896	393.995	3721.025	-41.354
4800	1164.017	3114.468	2126.705	4741.263	386.434	3791.955	-41.264
4900	1164.672	3138.476	2147.110	4857.698	378.421	3862.887	-41.178
5000	1165.290	3162.012	2167.173	4974.196	370.063	3934.202	-41.099

3.545. Dibenzo[*fg,ij*]naphtho[7,8,1,2,3-*pqrst*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-91-8
Point Group: C_s

Length: 15.89 Å
Width: 11.65 Å
Breadth: 3.887 Å
L/B Ratio: 1.365

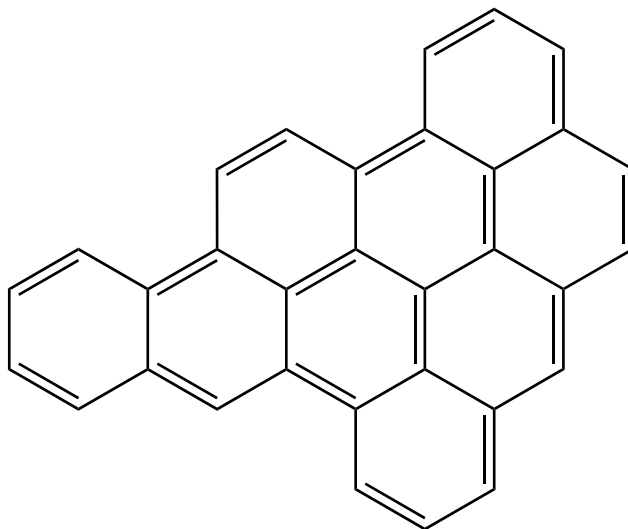
Cartesian coordinates:

C	3.1436	2.7906	0.0000	C	-2.8504	-1.5188	0.0000	H	4.2400	2.8902	0.0000
C	2.3343	3.9196	0.0000	C	-3.6696	-0.3776	0.0000	H	2.7881	4.9160	0.0000
C	0.9544	3.7870	0.0000	C	-5.0662	-0.5368	0.0000	H	0.3107	4.6799	0.0000
C	2.5814	1.5121	0.0000	C	-5.6375	-1.7947	0.0000	H	-1.0294	-3.5023	0.0000
C	-0.5751	-2.4982	0.0000	C	-4.8229	-2.9297	0.0000	H	-1.4649	4.5022	0.0000
C	-1.4001	-1.3780	0.0000	C	-3.4482	-2.7910	0.0000	H	-3.9407	4.2499	0.0000
C	-3.0728	0.9511	0.0000	C	3.4297	0.3277	0.0000	H	-4.9684	1.9846	0.0000
C	-1.9217	3.5007	0.0000	C	5.0362	-1.9764	0.0000	H	-5.7021	0.3618	0.0000
C	-3.3009	3.3613	0.0000	C	5.6149	-0.7196	0.0000	H	-6.7268	-1.9045	0.0000
C	-3.8734	2.0962	0.0000	C	4.8193	0.4255	0.0000	H	-5.2754	-3.9266	0.0000
C	-1.6672	1.0871	0.0000	C	3.6391	-2.1079	0.0000	H	-2.8007	-3.6812	0.0000
C	-0.8249	-0.0838	0.0000	C	2.8295	-0.9529	0.0000	H	5.6637	-2.8749	0.0000
C	0.5735	0.0596	0.0000	C	1.3998	-1.0867	0.0000	H	6.7053	-0.6185	0.0000
C	1.1753	1.3711	0.0000	C	0.8188	-2.3702	0.0000	H	5.2841	1.4235	0.0000
C	0.3581	2.5202	0.0000	C	1.6694	-3.5310	0.0000	H	1.1942	-4.5187	0.0000
C	-1.0901	2.3749	0.0000	C	3.0167	-3.4054	0.0000	H	3.6662	-4.2884	0.0000

Table 3.545: Table of thermodynamic data as a function of temperature for Dibenzofg,ijnaphtho[7,8,1,2,3-pqrst]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-55.957	471.970	471.970	∞
100	119.136	372.211	858.468	-48.626	498.800	545.207	-284.781
200	243.434	490.928	644.870	-30.788	484.653	597.252	-155.983
250	314.889	552.872	620.240	-16.842	477.960	626.174	-130.829
298.15	384.513	614.301	614.301	0.000	471.970	655.278	-114.800
300	387.158	616.688	614.309	0.714	471.747	656.413	-114.289
350	456.804	681.650	619.280	21.829	466.199	687.642	-102.623
400	521.569	746.938	631.157	46.312	461.362	719.604	-93.969
450	580.375	811.826	647.633	73.887	457.152	752.143	-87.305
500	633.015	875.752	667.259	104.247	453.480	785.144	-82.022
600	721.309	999.290	712.392	172.139	447.445	852.074	-74.178
700	790.973	1115.919	761.794	247.888	442.953	919.895	-68.642
800	846.602	1225.305	812.971	329.867	439.837	988.246	-64.524
900	891.702	1327.713	864.538	416.858	437.916	1056.906	-61.340
1000	928.769	1423.644	915.703	507.940	437.030	1125.738	-58.801
1100	959.578	1513.654	966.014	602.404	436.974	1194.630	-56.727
1200	985.423	1598.288	1015.212	699.691	437.605	1263.473	-54.996
1300	1007.275	1678.051	1063.162	799.356	438.733	1332.256	-53.530
1400	1025.877	1753.397	1109.799	901.038	440.223	1400.941	-52.269
1500	1041.811	1824.732	1155.104	1004.442	441.996	1469.513	-51.172
1600	1055.539	1892.418	1199.089	1109.327	443.912	1537.950	-50.208
1700	1067.430	1956.775	1241.782	1215.489	445.899	1606.238	-49.353
1800	1077.783	2018.088	1283.220	1322.761	447.875	1674.482	-48.591
1900	1086.840	2076.609	1323.449	1431.003	449.812	1742.556	-47.905
2000	1094.800	2132.563	1362.516	1540.093	451.655	1810.561	-47.286
2100	1101.827	2186.152	1400.470	1649.932	453.317	1878.461	-46.723
2200	1108.055	2237.555	1437.359	1760.432	454.801	1946.288	-46.210
2300	1113.597	2286.935	1473.231	1871.520	456.105	2014.054	-45.740
2400	1118.546	2334.436	1508.131	1983.131	457.149	2081.709	-45.306
2500	1122.983	2380.189	1542.104	2095.212	457.949	2149.458	-44.910
2600	1126.974	2424.312	1575.192	2207.713	458.467	2217.044	-44.540
2700	1130.574	2466.913	1607.434	2320.594	458.707	2284.704	-44.199
2800	1133.833	2508.089	1638.869	2433.817	458.642	2352.380	-43.883
2900	1136.790	2547.929	1669.533	2547.350	458.240	2420.005	-43.588
3000	1139.481	2586.514	1699.459	2661.166	457.551	2487.680	-43.313
3100	1141.937	2623.918	1728.680	2775.239	456.488	2555.292	-43.055
3200	1144.184	2660.209	1757.226	2889.546	455.100	2623.031	-42.816
3300	1146.244	2695.450	1785.126	3004.069	453.367	2690.866	-42.592
3400	1148.137	2729.697	1812.406	3118.789	451.255	2758.654	-42.381
3500	1149.881	2763.004	1839.092	3233.692	448.773	2826.490	-42.182
3600	1151.490	2795.420	1865.209	3348.761	445.947	2894.507	-41.997
3700	1152.977	2826.990	1890.778	3463.985	442.739	2962.622	-41.824
3800	1154.356	2857.757	1915.822	3579.353	439.123	3030.765	-41.660
3900	1155.635	2887.759	1940.360	3694.853	435.143	3098.942	-41.505
4000	1156.824	2917.032	1964.413	3810.477	430.782	3167.391	-41.361
4100	1157.931	2945.611	1987.997	3926.215	426.001	3235.868	-41.225
4200	1158.964	2973.526	2011.131	4042.061	420.830	3304.456	-41.096
4300	1159.929	3000.809	2033.831	4158.006	415.255	3373.067	-40.974
4400	1160.831	3027.486	2056.112	4274.044	409.286	3441.917	-40.860
4500	1161.676	3053.582	2077.989	4390.170	402.940	3510.971	-40.753
4600	1162.469	3079.123	2099.476	4506.378	396.155	3580.186	-40.653
4700	1163.214	3104.132	2120.587	4622.662	388.952	3649.418	-40.558
4800	1163.914	3128.629	2141.333	4739.019	381.381	3718.932	-40.469
4900	1164.573	3152.635	2161.728	4855.444	373.357	3788.448	-40.385
5000	1165.194	3176.169	2181.782	4971.932	364.990	3858.347	-40.307

3.546. Anthra[2,1,9,8-*defgh*]benzo[*rst*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-01-3
Point Group: C_s

Length: 15.91 Å
Width: 11.65 Å
Breadth: 3.888 Å
L/B Ratio: 1.366

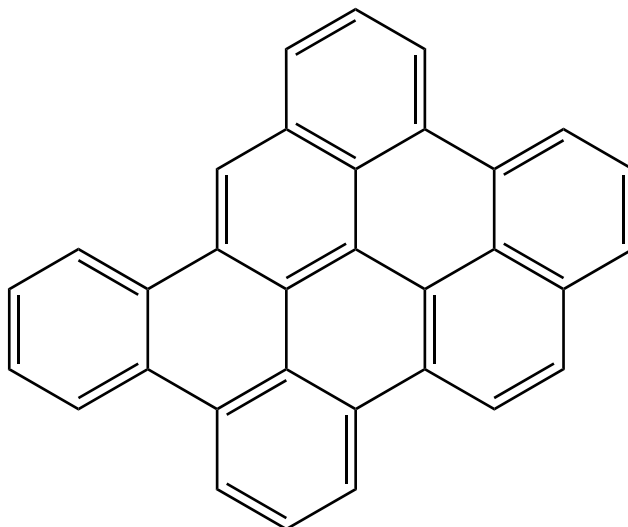
Cartesian coordinates:

C	3.1626	1.3137	0.0000	C	4.0936	0.2323	0.0000	H	3.5474	2.3467	0.0000
C	2.2023	-1.3355	0.0000	C	3.6235	-1.0930	0.0000	H	-0.0505	-3.9192	0.0000
C	0.3458	-2.8920	0.0000	C	4.5603	-2.1523	0.0000	H	2.4114	-3.4929	0.0000
C	1.6926	-2.6589	0.0000	C	5.9095	-1.8934	0.0000	H	-3.5389	3.6024	0.0000
C	-0.5776	-1.8166	0.0000	C	6.3771	-0.5658	0.0000	H	2.3869	3.7274	0.0000
C	-2.8397	2.7570	0.0000	C	5.4868	0.4805	0.0000	H	0.7725	5.6154	0.0000
C	-1.4480	3.0162	0.0000	C	-2.0044	-2.0695	0.0000	H	-1.6759	5.1782	0.0000
C	1.3058	3.5187	0.0000	C	-4.7774	-2.5190	0.0000	H	4.1809	-3.1856	0.0000
C	0.3897	4.5895	0.0000	C	-3.8897	-3.5917	0.0000	H	6.6306	-2.7172	0.0000
C	-0.9584	4.3499	0.0000	C	-2.5216	-3.3727	0.0000	H	7.4555	-0.3762	0.0000
C	0.8686	2.2097	0.0000	C	-4.2942	-1.2111	0.0000	H	5.8435	1.5167	0.0000
C	-0.5325	1.9401	0.0000	C	-2.8986	-0.9783	0.0000	H	-5.8580	-2.7014	0.0000
C	-1.0202	0.6046	0.0000	C	-2.3968	0.3668	0.0000	H	-4.2767	-4.6162	0.0000
C	-0.0969	-0.5037	0.0000	C	-3.3134	1.4619	0.0000	H	-1.8197	-4.2206	0.0000
C	1.3065	-0.2554	0.0000	C	-4.7328	1.1832	0.0000	H	-5.4198	2.0374	0.0000
C	1.8120	1.0930	0.0000	C	-5.1972	-0.0827	0.0000	H	-6.2735	-0.2904	0.0000

Table 3.546: Table of thermodynamic data as a function of temperature for Anthra[2,1,9,8-*defgh*]benzo[*rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.090	486.416	486.416	∞
100	118.928	367.369	855.964	-48.859	513.013	559.904	-292.458
200	244.740	486.420	641.246	-30.965	498.923	612.423	-159.945
250	316.737	548.719	616.474	-16.939	492.309	641.561	-134.044
298.15	386.659	610.501	610.501	0.000	486.416	670.857	-117.529
300	389.311	612.901	610.509	0.718	486.198	671.999	-117.003
350	459.068	678.206	615.507	21.945	480.761	703.409	-104.976
400	523.819	743.796	627.445	46.541	476.036	735.536	-96.049
450	582.540	808.945	643.999	74.225	471.937	768.224	-89.171
500	635.063	873.093	663.711	104.691	468.371	801.364	-83.716
600	723.107	996.982	709.023	172.776	462.528	868.541	-75.612
700	792.552	1113.872	758.596	248.693	458.205	936.579	-69.887
800	848.001	1223.456	809.930	330.821	455.237	1005.125	-65.627
900	892.955	1326.021	861.638	417.944	453.448	1073.962	-62.330
1000	929.900	1422.077	912.931	509.146	452.682	1142.957	-59.701
1100	960.604	1512.189	963.356	603.717	452.733	1212.000	-57.552
1200	986.358	1596.909	1012.658	701.102	453.462	1280.985	-55.759
1300	1008.128	1676.743	1060.700	800.856	454.680	1349.902	-54.239
1400	1026.657	1752.150	1107.422	902.619	456.251	1418.715	-52.932
1500	1042.527	1823.537	1152.804	1006.099	458.099	1487.409	-51.795
1600	1056.197	1891.267	1196.860	1111.052	460.084	1555.963	-50.796
1700	1068.036	1955.662	1239.617	1217.277	462.133	1624.365	-49.910
1800	1078.342	2017.008	1281.115	1324.608	464.168	1692.718	-49.120
1900	1087.357	2075.558	1321.399	1432.902	466.158	1760.899	-48.409
2000	1095.278	2131.538	1360.516	1542.043	468.051	1829.007	-47.768
2100	1102.270	2185.149	1398.517	1651.927	469.759	1897.009	-47.185
2200	1108.467	2236.573	1435.450	1762.470	471.286	1964.935	-46.653
2300	1113.981	2285.970	1471.362	1873.598	472.630	2032.798	-46.165
2400	1118.905	2333.487	1506.300	1985.247	473.711	2100.549	-45.716
2500	1123.318	2379.254	1540.309	2097.362	474.546	2168.392	-45.305
2600	1127.288	2423.390	1573.430	2209.896	475.096	2236.071	-44.922
2700	1130.869	2466.002	1605.703	2322.806	475.366	2303.822	-44.569
2800	1134.109	2507.189	1637.168	2436.058	475.330	2371.589	-44.242
2900	1137.050	2547.038	1667.859	2549.618	474.954	2439.304	-43.936
3000	1139.727	2585.632	1697.812	2663.459	474.291	2507.068	-43.651
3100	1142.169	2623.044	1727.058	2777.556	473.252	2574.768	-43.384
3200	1144.403	2659.342	1755.627	2891.886	471.886	2642.594	-43.135
3300	1146.451	2694.589	1783.549	3006.430	470.174	2710.515	-42.903
3400	1148.333	2728.842	1810.851	3121.171	468.083	2778.389	-42.684
3500	1150.067	2762.155	1837.557	3236.092	465.620	2846.310	-42.478
3600	1151.667	2794.576	1863.693	3351.180	462.812	2914.412	-42.286
3700	1153.146	2826.151	1889.280	3466.421	459.621	2982.611	-42.106
3800	1154.516	2856.922	1914.341	3581.805	456.021	3050.838	-41.936
3900	1155.788	2886.927	1938.896	3697.321	452.057	3119.098	-41.775
4000	1156.970	2916.204	1962.965	3812.960	447.712	3187.630	-41.625
4100	1158.071	2944.787	1986.564	3928.712	442.944	3256.189	-41.484
4200	1159.097	2972.706	2009.713	4044.571	437.787	3324.859	-41.350
4300	1160.056	2999.991	2032.426	4160.529	432.225	3393.552	-41.223
4400	1160.953	3026.671	2054.721	4276.580	426.268	3462.485	-41.104
4500	1161.793	3052.770	2076.611	4392.718	419.934	3531.620	-40.993
4600	1162.581	3078.314	2098.110	4508.937	413.161	3600.915	-40.889
4700	1163.321	3103.325	2119.233	4625.233	405.969	3670.228	-40.789
4800	1164.017	3127.824	2139.991	4741.600	398.408	3739.823	-40.697
4900	1164.673	3151.832	2160.396	4858.035	390.395	3809.419	-40.608
5000	1165.290	3175.368	2180.461	4974.533	382.037	3879.399	-40.527

3.547. Dibenzo[*cd,n*]naphtho[3,2,1,8-*pgra*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 109278-09-3
Point Group: C_s

Length: 15.92 Å
Width: 11.65 Å
Breadth: 3.891 Å
L/B Ratio: 1.366

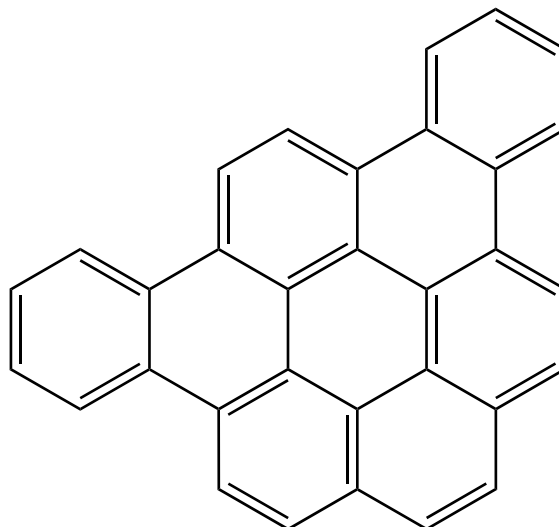
Cartesian coordinates:

C	-3.0045	-3.1096	0.0000	C	-1.0951	-1.6157	0.0000	H	-4.0949	-3.2627	0.0000
C	-2.1410	-4.2186	0.0000	C	-0.5373	-0.3023	0.0000	H	-2.5678	-5.2270	0.0000
C	-0.7802	-4.0396	0.0000	C	0.5463	2.3224	0.0000	H	-0.1022	-4.9005	0.0000
C	-0.2342	-2.7324	0.0000	C	3.3216	2.6838	0.0000	H	1.8349	-3.4101	0.0000
C	1.1705	-2.5307	0.0000	C	2.4714	3.7913	0.0000	H	-1.3340	4.2564	0.0000
C	-0.8856	2.1294	0.0000	C	1.1039	3.6150	0.0000	H	-3.7994	3.9377	0.0000
C	-1.7738	3.2472	0.0000	C	2.8073	1.3926	0.0000	H	-5.7448	2.4540	0.0000
C	-3.1231	3.0752	0.0000	C	1.4020	1.2009	0.0000	H	-6.7000	0.1571	0.0000
C	-3.6877	1.7637	0.0000	C	0.8483	-0.1248	0.0000	H	-5.1973	-1.8268	0.0000
C	-5.0883	1.5765	0.0000	C	1.7121	-1.2668	0.0000	H	4.4126	2.8302	0.0000
C	-5.6152	0.3065	0.0000	C	3.6931	0.2330	0.0000	H	2.8970	4.8002	0.0000
C	-4.7689	-0.8124	0.0000	C	3.1581	-1.0660	0.0000	H	0.4284	4.4839	0.0000
C	-1.4122	0.8401	0.0000	C	4.0306	-2.1656	0.0000	H	3.6051	-3.1809	0.0000
C	-2.8312	0.6444	0.0000	C	5.4023	-1.9853	0.0000	H	6.0705	-2.8525	0.0000
C	-3.3922	-0.6622	0.0000	C	5.9336	-0.6953	0.0000	H	7.0187	-0.5503	0.0000
C	-2.5045	-1.8203	0.0000	C	5.0869	0.3989	0.0000	H	5.5004	1.4191	0.0000

Table 3.547: Table of thermodynamic data as a function of temperature for Dibenzoc[cd,n]naphtho[3,2,1,8-pqra]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-56.076	485.902	485.902	∞
100	119.485	371.775	859.106	-48.733	512.625	559.075	-292.025
200	244.010	490.836	645.060	-30.845	498.529	611.146	-159.612
250	315.468	552.910	620.388	-16.870	491.865	640.069	-133.732
298.15	385.076	614.440	614.440	0.000	485.902	669.169	-117.233
300	387.720	616.830	614.447	0.715	485.681	670.304	-116.708
350	457.335	681.876	619.425	21.858	480.160	701.524	-104.695
400	522.064	747.233	631.317	46.366	475.348	733.473	-95.780
450	580.833	812.177	647.811	73.964	471.162	765.995	-88.913
500	633.438	876.149	667.456	104.347	467.513	798.978	-83.467
600	721.668	999.759	712.629	172.278	461.516	865.864	-75.379
700	791.280	1116.439	762.068	248.060	457.058	933.635	-69.667
800	846.866	1225.863	813.278	330.068	453.970	1001.932	-65.418
900	891.932	1328.301	864.874	417.084	452.074	1070.535	-62.131
1000	928.970	1424.254	916.066	508.187	451.209	1139.308	-59.510
1100	959.755	1514.282	966.400	602.670	451.172	1208.137	-57.368
1200	985.581	1598.931	1015.620	699.973	451.819	1276.917	-55.582
1300	1007.416	1678.705	1063.588	799.653	452.963	1345.635	-54.067
1400	1026.003	1754.061	1110.241	901.348	454.466	1414.254	-52.765
1500	1041.925	1825.405	1155.562	1004.765	456.251	1482.759	-51.633
1600	1055.642	1893.098	1199.560	1109.660	458.178	1551.128	-50.638
1700	1067.524	1957.461	1242.265	1215.832	460.174	1619.348	-49.755
1800	1077.869	2018.778	1283.715	1323.114	462.160	1687.523	-48.970
1900	1086.918	2077.304	1323.955	1431.363	464.105	1755.528	-48.262
2000	1094.872	2133.262	1363.031	1540.461	465.955	1823.463	-47.623
2100	1101.893	2186.854	1400.994	1650.306	467.624	1891.294	-47.042
2200	1108.116	2238.261	1437.891	1760.813	469.115	1959.050	-46.513
2300	1113.653	2287.643	1473.770	1871.907	470.425	2026.745	-46.028
2400	1118.599	2335.146	1508.678	1983.524	471.474	2094.330	-45.581
2500	1123.032	2380.901	1542.657	2095.609	472.279	2162.007	-45.172
2600	1127.019	2425.026	1575.751	2208.115	472.801	2229.522	-44.791
2700	1130.617	2467.629	1607.999	2321.000	473.046	2297.110	-44.439
2800	1133.872	2508.806	1639.440	2434.227	472.985	2364.715	-44.113
2900	1136.827	2548.648	1670.108	2547.765	472.587	2432.268	-43.809
3000	1139.516	2587.234	1700.039	2661.584	471.902	2499.872	-43.526
3100	1141.970	2624.639	1729.265	2775.660	470.842	2567.412	-43.260
3200	1144.215	2660.931	1757.815	2889.971	469.457	2635.078	-43.012
3300	1146.273	2696.173	1785.719	3004.497	467.727	2702.841	-42.782
3400	1148.165	2730.421	1813.003	3119.220	465.618	2770.557	-42.564
3500	1149.907	2763.729	1839.693	3234.125	463.139	2838.320	-42.359
3600	1151.514	2796.145	1865.813	3349.197	460.315	2906.265	-42.168
3700	1153.001	2827.716	1891.386	3464.424	457.110	2974.307	-41.989
3800	1154.378	2858.483	1916.432	3579.793	453.495	3042.377	-41.820
3900	1155.656	2888.486	1940.974	3695.296	449.518	3110.482	-41.659
4000	1156.844	2917.759	1965.029	3810.922	445.160	3178.858	-41.511
4100	1157.951	2946.339	1988.616	3926.662	440.380	3247.262	-41.370
4200	1158.983	2974.255	2011.753	4042.509	435.211	3315.777	-41.237
4300	1159.946	3001.538	2034.455	4158.456	429.638	3384.315	-41.110
4400	1160.848	3028.215	2056.738	4274.497	423.671	3453.093	-40.993
4500	1161.693	3054.312	2078.618	4390.624	417.326	3522.074	-40.882
4600	1162.485	3079.854	2100.107	4506.833	410.543	3591.216	-40.779
4700	1163.229	3104.862	2121.220	4623.119	403.341	3660.375	-40.680
4800	1163.928	3129.360	2141.968	4739.478	395.772	3729.815	-40.588
4900	1164.587	3153.366	2162.365	4855.904	387.750	3799.258	-40.500
5000	1165.208	3176.900	2182.421	4972.394	379.384	3869.084	-40.419

3.548. Dibenzo[*a,g*]coronene



Formula: $C_{32}H_{16}$
Mass: 400.469 g/mol
CAS Number: 190-66-9
Point Group: C_{2v}

Length: 15.92 Å
Width: 11.64 Å
Breadth: 3.885 Å
L/B Ratio: 1.367

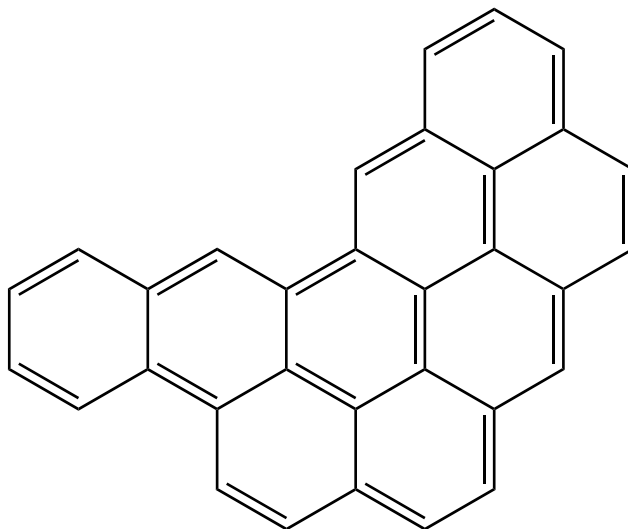
Cartesian coordinates:

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C	-1.4270	-1.7493	0.0000	C	-3.4952	1.9857	0.0000	H	1.2107	-3.9317	0.0000
C	-0.7128	-2.9662	0.0000	C	-2.8255	0.7380	0.0000	H	4.6308	1.9037	0.0000
C	0.6600	-2.9784	0.0000	C	-1.4270	0.7122	0.0000	H	3.4009	4.0651	0.0000
C	0.7058	-0.5539	0.0000	C	-2.8771	-1.7331	0.0000	H	1.2895	5.3078	0.0000
C	1.3957	-1.7744	0.0000	C	-3.5666	-0.5078	0.0000	H	-1.1948	5.3299	0.0000
C	1.4394	0.6867	0.0000	C	-4.9762	-0.5131	0.0000	H	-3.3280	4.1250	0.0000
C	2.8381	0.6876	0.0000	C	-5.6789	-1.6984	0.0000	H	-4.5962	1.9859	0.0000
C	3.5300	1.9231	0.0000	C	-4.9919	-2.9197	0.0000	H	-5.5062	0.4517	0.0000
C	2.8540	3.1153	0.0000	C	-3.6140	-2.9348	0.0000	H	-6.7737	-1.6912	0.0000
C	0.7336	1.9217	0.0000	C	3.5569	-0.5712	0.0000	H	-5.5542	-3.8590	0.0000
C	1.4394	3.1357	0.0000	C	2.8458	-1.7840	0.0000	H	-3.0652	-3.8891	0.0000
C	0.7181	4.3725	0.0000	C	3.5612	-2.9986	0.0000	H	2.9955	-3.9430	0.0000
C	-0.6402	4.3846	0.0000	C	4.9391	-3.0080	0.0000	H	5.4847	-3.9572	0.0000
C	-0.6993	1.9345	0.0000	C	5.6477	-1.7991	0.0000	H	6.7425	-1.8113	0.0000
C	-1.3833	3.1609	0.0000	C	4.9662	-0.6015	0.0000	H	5.5133	0.3537	0.0000

Table 3.548: Table of thermodynamic data as a function of temperature for Dibenzo[*a,g*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-55.714	455.997	455.997	∞
100	118.124	357.483	843.175	-48.569	482.884	530.764	-277.237
200	243.182	475.694	629.695	-30.800	468.669	584.314	-152.604
250	315.036	537.627	605.051	-16.856	461.973	613.998	-128.285
298.15	384.936	599.107	599.107	0.000	455.997	643.836	-112.795
300	387.589	601.496	599.114	0.715	455.776	644.999	-112.302
350	457.410	666.539	604.091	21.857	450.254	676.986	-101.032
400	522.271	731.915	615.984	46.372	445.449	709.701	-92.676
450	581.118	796.888	632.481	73.983	441.276	742.989	-86.242
500	633.765	860.893	652.132	104.380	437.642	776.735	-81.143
600	722.024	984.565	697.321	172.346	431.680	845.144	-73.575
700	791.628	1101.301	746.781	248.164	427.257	914.431	-68.234
800	847.195	1210.769	798.013	330.206	424.203	984.240	-64.263
900	892.238	1313.245	849.630	417.253	422.338	1054.350	-61.192
1000	929.253	1409.229	900.843	508.386	421.503	1124.627	-58.743
1100	960.016	1499.283	951.196	602.896	421.493	1194.957	-56.743
1200	985.821	1583.954	1000.433	700.225	422.166	1265.236	-55.073
1300	1007.636	1663.747	1048.418	799.927	423.333	1335.451	-53.658
1400	1026.206	1739.118	1095.087	901.644	424.857	1405.565	-52.441
1500	1042.112	1810.475	1140.422	1005.080	426.661	1475.564	-51.383
1600	1055.814	1878.180	1184.435	1109.993	428.606	1545.425	-50.452
1700	1067.683	1942.553	1227.152	1216.182	430.619	1615.136	-49.626
1800	1078.015	2003.879	1268.613	1323.478	432.619	1684.802	-48.891
1900	1087.054	2062.412	1308.864	1431.742	434.579	1754.296	-48.228
2000	1094.998	2118.377	1347.951	1540.853	436.442	1823.720	-47.630
2100	1102.010	2171.975	1385.923	1650.710	438.123	1893.039	-47.086
2200	1108.224	2223.387	1422.829	1761.228	439.625	1962.283	-46.590
2300	1113.754	2272.774	1458.716	1872.332	440.945	2031.465	-46.135
2400	1118.693	2320.281	1493.631	1983.959	442.004	2100.536	-45.716
2500	1123.120	2366.040	1527.618	2096.054	442.819	2169.700	-45.332
2600	1127.102	2410.168	1560.719	2208.568	443.350	2238.701	-44.975
2700	1130.694	2452.774	1592.973	2321.461	443.603	2307.774	-44.646
2800	1133.945	2493.954	1624.420	2434.696	443.549	2376.864	-44.340
2900	1136.896	2533.798	1655.095	2548.240	443.158	2445.902	-44.055
3000	1139.581	2572.387	1685.031	2662.066	442.480	2514.991	-43.789
3100	1142.032	2609.794	1714.262	2776.149	441.426	2584.016	-43.539
3200	1144.273	2646.088	1742.817	2890.466	440.047	2653.167	-43.308
3300	1146.328	2681.331	1770.726	3004.997	438.322	2722.414	-43.091
3400	1148.217	2715.581	1798.014	3119.726	436.219	2791.614	-42.887
3500	1149.956	2748.890	1824.709	3234.636	433.745	2860.861	-42.695
3600	1151.561	2781.308	1850.833	3349.712	430.926	2930.289	-42.517
3700	1153.046	2812.880	1876.409	3464.944	427.725	2999.816	-42.349
3800	1154.421	2843.649	1901.460	3580.318	424.115	3069.369	-42.191
3900	1155.697	2873.652	1926.005	3695.825	420.142	3138.957	-42.041
4000	1156.883	2902.927	1950.063	3811.454	415.787	3208.817	-41.902
4100	1157.988	2931.507	1973.654	3927.198	411.012	3278.704	-41.770
4200	1159.018	2959.424	1996.793	4043.049	405.847	3348.702	-41.646
4300	1159.980	2986.708	2019.499	4159.000	400.277	3418.723	-41.528
4400	1160.880	3013.386	2041.785	4275.043	394.312	3488.984	-41.419
4500	1161.724	3039.483	2063.667	4391.174	387.971	3559.448	-41.316
4600	1162.514	3065.026	2085.159	4507.386	381.191	3630.072	-41.220
4700	1163.257	3090.035	2106.274	4623.675	373.992	3700.714	-41.128
4800	1163.956	3114.533	2127.025	4740.036	366.425	3771.637	-41.043
4900	1164.613	3138.540	2147.424	4856.465	358.406	3842.563	-40.961
5000	1165.233	3162.074	2167.483	4972.958	350.043	3913.872	-40.887

3.549. Dibenzo[*ghi,n*]naphtho[8,1,2-*bcd*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-05-7
Point Group: C_s

Length: 15.93 Å
Width: 11.62 Å
Breadth: 3.886 Å
L/B Ratio: 1.371

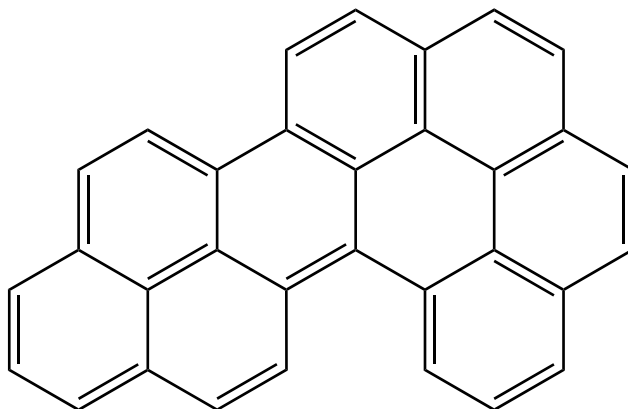
Cartesian coordinates:

C	1.8925	-1.8937	0.0000	C	-2.4085	-2.1776	0.0000	H	1.4173	-2.8884	0.0000
C	3.1304	0.6390	0.0000	C	-5.2113	-2.3212	0.0000	H	4.8275	1.9888	0.0000
C	3.7280	1.9306	0.0000	C	-4.4417	-3.4866	0.0000	H	3.4324	4.0530	0.0000
C	2.9647	3.0619	0.0000	C	-3.0599	-3.4234	0.0000	H	1.2380	5.1262	0.0000
C	1.5463	2.9716	0.0000	C	-3.1798	-0.9959	0.0000	H	-1.2398	4.9677	0.0000
C	0.7371	4.1512	0.0000	C	-2.5274	0.2764	0.0000	H	-3.2756	3.6239	0.0000
C	-0.6189	4.0645	0.0000	C	-3.3077	1.4699	0.0000	H	-0.3862	-3.0056	0.0000
C	-1.2722	2.7901	0.0000	C	-4.7492	1.3562	0.0000	H	-6.3050	-2.3895	0.0000
C	-2.6810	2.7019	0.0000	C	-5.3591	0.1523	0.0000	H	-4.9422	-4.4608	0.0000
C	-0.9819	-2.0782	0.0000	C	-4.5945	-1.0737	0.0000	H	-2.4639	-4.3429	0.0000
C	1.7339	0.5280	0.0000	C	3.9430	-0.5502	0.0000	H	-5.3329	2.2841	0.0000
C	0.9364	1.7117	0.0000	C	3.3163	-1.8097	0.0000	H	-6.4523	0.0721	0.0000
C	-0.4945	1.6174	0.0000	C	4.1072	-2.9841	0.0000	H	3.6101	-3.9607	0.0000
C	-1.1260	0.3480	0.0000	C	5.4776	-2.8969	0.0000	H	6.0911	-3.8038	0.0000
C	-0.3488	-0.8648	0.0000	C	6.1076	-1.6375	0.0000	H	7.2011	-1.5839	0.0000
C	1.1115	-0.7689	0.0000	C	5.3565	-0.4879	0.0000	H	5.8353	0.5032	0.0000

Table 3.549: Table of thermodynamic data as a function of temperature for Dibenzo[ghi,n]naphtho[8,1,2-bcd]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.532	477.037	477.037	∞
100	116.745	361.429	846.695	-48.527	503.967	551.452	-288.043
200	243.080	479.090	633.239	-30.830	489.680	604.646	-157.914
250	315.381	541.052	608.567	-16.879	482.991	634.160	-132.498
298.15	385.491	602.614	602.614	0.000	477.037	663.830	-116.298
300	388.149	605.007	602.621	0.716	476.817	664.987	-115.782
350	458.019	670.141	607.606	21.887	471.325	696.796	-103.989
400	522.842	735.596	619.515	46.433	466.550	729.329	-95.239
450	581.623	800.633	636.032	74.070	462.404	762.431	-88.499
500	634.205	864.688	655.705	104.491	458.793	795.989	-83.155
600	722.373	988.432	700.938	172.496	452.870	864.014	-75.218
700	791.946	1105.218	750.437	248.347	448.480	932.913	-69.613
800	847.515	1214.729	801.704	330.420	445.458	1002.327	-65.444
900	892.571	1317.243	853.353	417.500	443.626	1072.039	-62.218
1000	929.600	1413.263	904.595	508.668	442.825	1141.914	-59.646
1100	960.372	1503.350	954.975	603.212	442.850	1211.840	-57.544
1200	986.178	1588.052	1004.238	700.577	443.558	1281.710	-55.790
1300	1007.990	1667.874	1052.247	800.315	444.760	1351.514	-54.303
1400	1026.551	1743.271	1098.938	902.067	446.320	1421.214	-53.025
1500	1042.445	1814.652	1144.294	1005.536	448.158	1490.796	-51.913
1600	1056.134	1882.377	1188.326	1110.482	450.136	1560.239	-50.936
1700	1067.988	1946.769	1231.062	1216.702	452.180	1629.530	-50.068
1800	1078.306	2008.112	1272.541	1324.029	454.210	1698.773	-49.296
1900	1087.330	2066.661	1312.808	1432.320	456.198	1767.843	-48.600
2000	1095.259	2122.639	1351.910	1541.458	458.088	1836.841	-47.972
2100	1102.256	2176.250	1389.897	1651.341	459.794	1905.733	-47.402
2200	1108.457	2227.673	1426.817	1761.883	461.320	1974.549	-46.881
2300	1113.974	2277.070	1462.718	1873.010	462.663	2043.302	-46.404
2400	1118.901	2324.586	1497.645	1984.658	463.743	2111.943	-45.964
2500	1123.317	2370.353	1531.644	2096.773	464.578	2180.676	-45.562
2600	1127.288	2414.489	1564.756	2209.306	465.128	2249.246	-45.187
2700	1130.870	2457.101	1597.021	2322.217	465.399	2317.887	-44.841
2800	1134.111	2498.288	1628.478	2435.469	465.363	2386.543	-44.521
2900	1137.053	2538.138	1659.162	2549.030	464.987	2455.148	-44.221
3000	1139.731	2576.731	1689.108	2662.871	464.324	2523.802	-43.942
3100	1142.173	2614.143	1718.347	2776.968	463.285	2592.392	-43.681
3200	1144.407	2650.442	1746.911	2891.299	461.920	2661.108	-43.437
3300	1146.456	2685.689	1774.827	3005.843	460.209	2729.920	-43.210
3400	1148.338	2719.942	1802.123	3120.584	458.118	2798.684	-42.996
3500	1150.072	2753.255	1828.825	3235.506	455.655	2867.495	-42.794
3600	1151.672	2785.676	1854.956	3350.594	452.848	2936.486	-42.606
3700	1153.151	2817.251	1880.539	3465.836	449.658	3005.575	-42.430
3800	1154.521	2848.022	1905.596	3581.221	446.058	3074.692	-42.264
3900	1155.793	2878.028	1930.147	3696.737	442.095	3143.842	-42.106
4000	1156.975	2907.305	1954.211	3812.376	437.750	3213.264	-41.960
4100	1158.076	2935.888	1977.808	3928.130	432.983	3282.713	-41.821
4200	1159.102	2963.807	2000.953	4043.989	427.827	3352.273	-41.691
4300	1160.061	2991.093	2023.663	4159.948	422.265	3421.856	-41.566
4400	1160.958	3017.772	2045.954	4275.999	416.309	3491.678	-41.451
4500	1161.798	3043.872	2067.841	4392.138	409.975	3561.703	-41.342
4600	1162.586	3069.416	2089.338	4508.357	403.203	3631.889	-41.241
4700	1163.326	3094.427	2110.458	4624.653	396.011	3702.091	-41.143
4800	1164.022	3118.926	2131.213	4741.021	388.450	3772.576	-41.053
4900	1164.677	3142.934	2151.616	4857.456	380.438	3843.062	-40.967
5000	1165.295	3166.470	2171.679	4973.955	372.081	3913.931	-40.888

3.550. Benzo[*lm*]phenanthro[5,4,3-*abcd*]perylene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 109278-08-2
Point Group: C₁

Length: 15.88 Å
Width: 11.62 Å
Breadth: 4.981 Å
L/B Ratio: 1.366

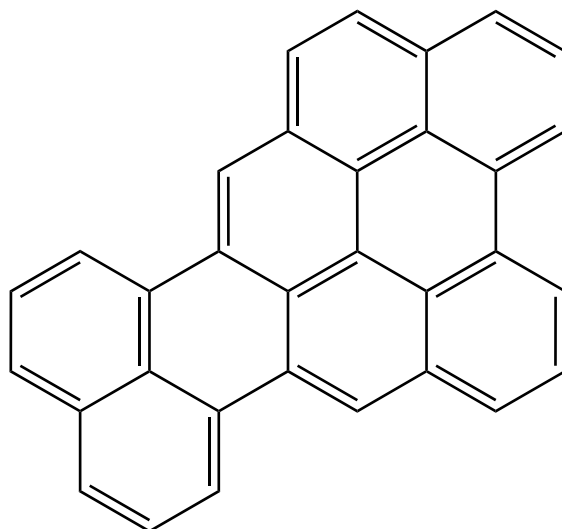
Cartesian coordinates:

C	-4.5053	-0.8915	0.1373	C	1.3538	-3.5941	0.0702	H	4.1216	4.2053	0.4198
C	-5.8670	-0.5582	0.0934	C	0.0479	-3.2508	0.1943	H	-0.0198	3.1523	0.8440
C	-6.2602	0.7451	-0.1626	C	2.9826	-0.2300	-0.1152	H	1.7714	4.8165	0.9716
C	-5.3101	1.7392	-0.3871	C	4.3246	-0.5942	-0.2893	H	5.7699	2.5092	-0.1785
C	-3.9512	1.4325	-0.3438	C	4.6748	-1.9655	-0.3735	H	6.3684	0.1229	-0.5288
C	-3.5311	0.1101	-0.0684	C	3.7149	-2.9330	-0.2535	H	5.7262	-2.2361	-0.5232
C	-2.1322	-0.2104	-0.0015	C	2.6207	1.1465	0.0415	H	3.9840	-3.9945	-0.3006
C	-1.1518	0.8190	-0.1273	C	3.6432	2.1160	0.0831	H	1.6654	-4.6448	0.0712
C	-1.6309	2.1319	-0.4960	C	5.0026	1.7267	-0.1581	H	-0.7289	-4.0228	0.3060
C	-2.9436	2.4283	-0.5993	C	5.3304	0.4240	-0.3467	H	-3.2739	3.4317	-0.8922
C	-1.7496	-1.5465	0.1996	C	1.2600	1.5229	0.2196	H	-0.8880	2.9103	-0.7196
C	-0.3714	-1.8805	0.1681	C	1.0038	2.8352	0.6019	H	-6.6181	-1.3383	0.2620
C	0.5931	-0.8564	0.0865	C	2.0232	3.7907	0.6820	H	-7.3252	0.9980	-0.1936
C	0.2066	0.5164	0.0604	C	3.3259	3.4526	0.3908	H	-5.6305	2.7652	-0.6005
C	1.9763	-1.2314	-0.0237	C	-4.0770	-2.2393	0.3821	H	-2.4247	-3.5838	0.5680
C	2.3532	-2.5812	-0.0684	C	-2.7592	-2.5489	0.3993	H	-4.8412	-3.0076	0.5461

Table 3.550: Table of thermodynamic data as a function of temperature for Benzo[*lm*]phenanthro[5,4,3-*abcd*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.276	499.248	499.248	∞
100	114.815	357.415	841.611	-48.420	526.284	574.171	-299.910
200	242.692	474.182	628.394	-30.842	511.877	627.825	-163.968
250	315.553	536.122	603.704	-16.896	505.184	657.586	-137.392
298.15	385.998	597.745	597.745	0.000	499.248	687.492	-120.443
300	388.666	600.141	597.752	0.717	499.028	688.658	-119.904
350	458.742	665.372	602.744	21.920	493.568	720.708	-107.558
400	523.680	730.932	614.671	46.504	488.832	753.477	-98.392
450	582.514	796.071	631.214	74.186	484.729	786.809	-91.329
500	635.105	860.221	650.918	104.652	481.163	820.593	-85.725
600	723.215	984.124	696.217	172.744	475.328	889.057	-77.398
700	792.683	1101.032	745.784	248.674	471.017	958.379	-71.514
800	848.137	1210.635	797.116	330.815	468.063	1028.208	-67.134
900	893.088	1313.215	848.824	417.952	466.288	1098.326	-63.744
1000	930.026	1409.285	900.119	509.166	465.534	1168.601	-61.040
1100	960.723	1499.409	950.546	603.750	465.598	1238.922	-58.830
1200	986.468	1584.139	999.851	701.146	466.338	1309.185	-56.986
1300	1008.230	1663.982	1047.897	800.911	467.567	1379.379	-55.423
1400	1026.752	1739.396	1094.621	902.684	469.148	1449.468	-54.079
1500	1042.614	1810.789	1140.007	1006.173	471.005	1519.437	-52.910
1600	1056.278	1878.525	1184.066	1111.134	472.998	1589.265	-51.883
1700	1068.111	1942.925	1226.826	1217.367	475.055	1658.941	-50.972
1800	1078.411	2004.274	1268.327	1324.705	477.097	1728.568	-50.161
1900	1087.421	2062.828	1308.614	1433.007	479.094	1798.021	-49.430
2000	1095.338	2118.811	1347.734	1542.153	480.993	1867.403	-48.771
2100	1102.325	2172.425	1385.738	1652.043	482.707	1936.677	-48.171
2200	1108.518	2223.851	1422.673	1762.591	484.239	2005.876	-47.625
2300	1114.028	2273.251	1458.588	1873.724	485.588	2075.011	-47.124
2400	1118.949	2320.769	1493.528	1985.378	486.673	2144.034	-46.663
2500	1123.360	2366.538	1527.539	2097.497	487.513	2213.148	-46.240
2600	1127.327	2410.676	1560.662	2210.035	488.067	2282.099	-45.847
2700	1130.905	2453.289	1592.938	2322.949	488.341	2351.121	-45.484
2800	1134.144	2494.477	1624.404	2436.204	488.308	2420.159	-45.148
2900	1137.083	2534.328	1655.098	2549.768	487.936	2489.145	-44.833
3000	1139.757	2572.923	1685.052	2663.612	487.276	2558.180	-44.541
3100	1142.198	2610.335	1714.299	2777.712	486.239	2627.151	-44.266
3200	1144.430	2646.634	1742.871	2892.045	484.877	2696.248	-44.011
3300	1146.477	2681.882	1770.794	3006.592	483.167	2765.440	-43.772
3400	1148.358	2716.136	1798.097	3121.335	481.078	2834.584	-43.547
3500	1150.090	2749.450	1824.805	3236.258	478.618	2903.776	-43.336
3600	1151.688	2781.871	1850.941	3351.348	475.812	2973.148	-43.138
3700	1153.167	2813.447	1876.530	3466.592	472.624	3042.618	-42.953
3800	1154.536	2844.218	1901.593	3581.978	469.026	3112.114	-42.778
3900	1155.807	2874.225	1926.149	3697.496	465.063	3181.645	-42.612
4000	1156.988	2903.502	1950.218	3813.136	460.720	3251.447	-42.459
4100	1158.088	2932.085	1973.819	3928.891	455.954	3321.277	-42.313
4200	1159.114	2960.004	1996.968	4044.751	450.799	3391.217	-42.175
4300	1160.072	2987.290	2019.683	4160.711	445.239	3461.180	-42.044
4400	1160.968	3013.970	2041.978	4276.764	439.283	3531.383	-41.922
4500	1161.808	3040.070	2063.869	4392.903	432.951	3601.788	-41.808
4600	1162.595	3065.614	2085.370	4509.123	426.179	3672.354	-41.700
4700	1163.335	3090.625	2106.493	4625.420	418.988	3742.936	-41.597
4800	1164.030	3115.124	2127.252	4741.789	411.429	3813.801	-41.502
4900	1164.685	3139.133	2147.658	4858.225	403.417	3884.667	-41.410
5000	1165.302	3162.669	2167.724	4974.725	395.060	3955.916	-41.326

3.551. Dibenzo[*de,ij*]naphtho[7,8,1,2,3-*pqrst*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-00-2
Point Group: C_s

Length: 15.94 Å
Width: 11.65 Å
Breadth: 3.886 Å
L/B Ratio: 1.368

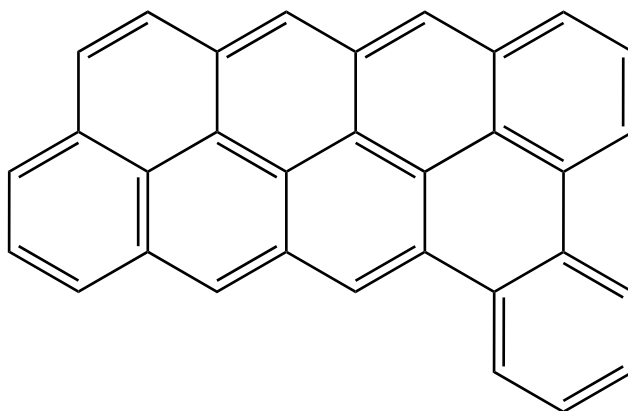
Cartesian coordinates:

C	-5.0161	0.5108	0.0000	C	-3.6293	0.4253	0.0000	H	-5.4886	1.5053	0.0000
C	-5.8031	-0.6446	0.0000	C	-3.0146	-0.8519	0.0000	H	-6.8942	-0.5514	0.0000
C	-5.2147	-1.8933	0.0000	C	-1.5859	-0.9771	0.0000	H	-5.8326	-2.7983	0.0000
C	-3.8127	-2.0139	0.0000	C	0.6329	0.0596	0.0000	H	-3.8187	-4.1929	0.0000
C	-3.1794	-3.3025	0.0000	C	1.2207	-1.2374	0.0000	H	-1.3440	-4.3984	0.0000
C	-1.8280	-3.4151	0.0000	C	1.4466	1.2476	0.0000	H	0.8750	-3.3588	0.0000
C	-0.9939	-2.2473	0.0000	C	2.6776	-1.3678	0.0000	H	1.4813	3.3879	0.0000
C	0.4129	-2.3581	0.0000	C	3.2847	-2.6070	0.0000	H	-0.5242	4.7980	0.0000
C	0.8549	2.4809	0.0000	C	4.6883	-2.7284	0.0000	H	-3.0001	5.0212	0.0000
C	-0.5663	2.6301	0.0000	C	5.4798	-1.6110	0.0000	H	-4.4457	2.9929	0.0000
C	-1.1621	3.9070	0.0000	C	3.4850	-0.1915	0.0000	H	2.6624	-3.5151	0.0000
C	-2.5359	4.0294	0.0000	C	4.8907	-0.3191	0.0000	H	5.1355	-3.7279	0.0000
C	-3.3493	2.8914	0.0000	C	5.7029	0.8461	0.0000	H	6.5723	-1.6963	0.0000
C	-0.7650	0.1846	0.0000	C	5.1259	2.0875	0.0000	H	6.7929	0.7330	0.0000
C	-1.3804	1.4803	0.0000	C	3.7230	2.2207	0.0000	H	5.7455	2.9902	0.0000
C	-2.7921	1.6190	0.0000	C	2.9029	1.1111	0.0000	H	3.2734	3.2257	0.0000

Table 3.551: Table of thermodynamic data as a function of temperature for Dibenzo[*de,ij*]naphtho[7,8,1,2,3-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.770	490.805	490.805	∞
100	118.023	368.041	854.086	-48.605	517.656	564.480	-294.848
200	243.403	486.331	640.444	-30.823	503.454	616.972	-161.133
250	315.274	548.316	615.783	-16.867	496.770	646.123	-134.997
298.15	385.135	609.835	609.835	0.000	490.805	675.445	-118.333
300	387.786	612.226	609.842	0.715	490.584	676.588	-117.802
350	457.535	677.294	614.822	21.865	485.070	708.038	-105.667
400	522.320	742.681	626.718	46.385	480.270	740.215	-96.660
450	581.105	807.656	643.220	73.997	476.098	772.964	-89.721
500	633.707	871.658	662.873	104.392	472.461	806.172	-84.219
600	721.926	995.315	708.065	172.350	466.491	873.505	-76.044
700	791.536	1112.035	757.524	248.158	462.059	941.719	-70.270
800	847.129	1221.493	808.754	330.191	458.996	1010.454	-65.975
900	892.203	1323.963	860.370	417.234	457.127	1079.492	-62.651
1000	929.247	1419.945	911.580	508.365	456.290	1148.697	-60.001
1100	960.034	1509.999	961.931	602.875	456.280	1217.956	-57.835
1200	985.857	1594.673	1011.167	700.207	456.956	1287.163	-56.028
1300	1007.685	1674.469	1059.151	799.914	458.127	1356.306	-54.496
1400	1026.263	1749.845	1105.819	901.636	459.657	1425.348	-53.179
1500	1042.174	1821.206	1151.154	1005.078	461.467	1494.274	-52.034
1600	1055.880	1888.914	1195.166	1109.997	463.418	1563.062	-51.028
1700	1067.749	1953.291	1237.884	1216.192	465.437	1631.700	-50.135
1800	1078.082	2014.621	1279.346	1323.496	467.445	1700.291	-49.340
1900	1087.120	2073.158	1319.597	1431.766	469.411	1768.711	-48.624
2000	1095.062	2129.126	1358.684	1540.883	471.280	1837.060	-47.978
2100	1102.072	2182.727	1396.657	1650.747	472.968	1905.304	-47.391
2200	1108.284	2234.142	1433.564	1761.271	474.476	1973.472	-46.855
2300	1113.812	2283.532	1469.453	1872.381	475.802	2041.579	-46.365
2400	1118.749	2331.041	1504.369	1984.014	476.867	2109.574	-45.913
2500	1123.174	2376.802	1538.357	2096.114	477.687	2177.662	-45.499
2600	1127.153	2420.933	1571.458	2208.634	478.223	2245.586	-45.113
2700	1130.743	2463.540	1603.714	2321.531	478.480	2313.583	-44.758
2800	1133.992	2504.722	1635.161	2434.771	478.432	2381.596	-44.428
2900	1136.940	2544.568	1665.837	2548.320	478.045	2449.558	-44.120
3000	1139.623	2583.158	1695.775	2662.150	477.371	2517.569	-43.834
3100	1142.072	2620.566	1725.006	2776.237	476.322	2585.517	-43.565
3200	1144.311	2656.862	1753.562	2890.557	474.946	2653.591	-43.315
3300	1146.365	2692.106	1781.472	3005.093	473.226	2721.760	-43.081
3400	1148.252	2726.357	1808.761	3119.825	471.126	2789.883	-42.860
3500	1149.990	2759.667	1835.456	3234.738	468.655	2858.052	-42.653
3600	1151.593	2792.086	1861.581	3349.818	465.839	2926.403	-42.460
3700	1153.076	2823.659	1887.158	3465.053	462.642	2994.851	-42.279
3800	1154.450	2854.428	1912.210	3580.430	459.035	3063.327	-42.107
3900	1155.725	2884.432	1936.755	3695.939	455.064	3131.837	-41.945
4000	1156.910	2913.708	1960.815	3811.572	450.713	3200.618	-41.795
4100	1158.014	2942.288	1984.406	3927.319	445.940	3269.427	-41.652
4200	1159.043	2970.206	2007.546	4043.172	440.777	3338.348	-41.518
4300	1160.004	2997.491	2030.252	4159.125	435.210	3407.290	-41.390
4400	1160.903	3024.169	2052.539	4275.171	429.248	3476.473	-41.270
4500	1161.746	3050.267	2074.422	4391.304	422.909	3545.858	-41.158
4600	1162.536	3075.810	2095.915	4507.518	416.131	3615.404	-41.053
4700	1163.278	3100.820	2117.030	4623.809	408.934	3684.968	-40.953
4800	1163.976	3125.318	2137.782	4740.172	401.369	3754.813	-40.860
4900	1164.632	3149.325	2158.182	4856.603	393.352	3824.660	-40.771
5000	1165.252	3172.860	2178.241	4973.098	384.991	3894.890	-40.689

3.552. Anthra[3,2,1,9,8-*rstuva*]benzo[*ij*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-16-0
Point Group: C_s

Length: 16.06 Å
Width: 11.38 Å
Breadth: 3.887 Å
L/B Ratio: 1.412

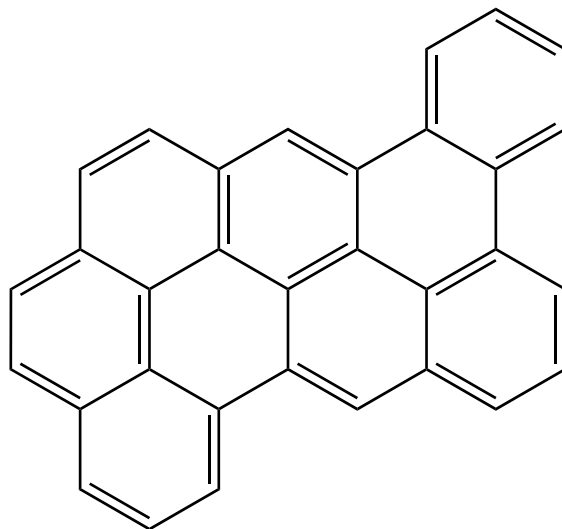
Cartesian coordinates:

C	5.0837	1.6830	0.0000	C	2.4946	0.5290	0.0000	H	6.1003	2.0932	0.0000
C	4.0082	2.4933	0.0000	C	2.1589	-2.2695	0.0000	H	4.1227	3.5836	0.0000
C	2.6578	1.9623	0.0000	C	1.0463	-1.4459	0.0000	H	1.6785	3.8692	0.0000
C	1.5629	2.7782	0.0000	C	1.2099	-0.0274	0.0000	H	-0.7551	4.1529	0.0000
C	0.2330	2.2363	0.0000	C	0.0587	0.8189	0.0000	H	-3.1738	4.4542	0.0000
C	-0.8794	3.0628	0.0000	C	-0.2863	-1.9812	0.0000	H	-5.4619	3.4829	0.0000
C	-2.1803	2.5190	0.0000	C	-1.3863	-1.1736	0.0000	H	-5.7848	1.0210	0.0000
C	-3.3222	3.3684	0.0000	C	-1.2294	0.2632	0.0000	H	4.4848	-3.6391	0.0000
C	-4.5806	2.8330	0.0000	C	-2.3610	1.1145	0.0000	H	6.7562	-2.6384	0.0000
C	-4.7643	1.4340	0.0000	C	-3.6852	0.5766	0.0000	H	7.0551	-0.1803	0.0000
C	4.9445	0.2400	0.0000	C	-2.7404	-1.7257	0.0000	H	2.0379	-3.3598	0.0000
C	4.6151	-2.5510	0.0000	C	-3.8591	-0.8739	0.0000	H	-0.4098	-3.0765	0.0000
C	5.8691	-1.9961	0.0000	C	-5.1450	-1.4323	0.0000	H	-6.0153	-0.7579	0.0000
C	6.0416	-0.5971	0.0000	C	-5.3246	-2.8057	0.0000	H	-6.3351	-3.2269	0.0000
C	3.4620	-1.7220	0.0000	C	-4.2162	-3.6505	0.0000	H	-4.3546	-4.7365	0.0000
C	3.6308	-0.3175	0.0000	C	-2.9394	-3.1136	0.0000	H	-2.0595	-3.7754	0.0000

Table 3.552: Table of thermodynamic data as a function of temperature for Anthra[3,2,1,9,8-*rstuva*]benzo[*ij*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-56.068	509.619	509.619	∞
100	118.218	367.416	856.312	-48.890	536.185	583.072	-304.559
200	244.951	486.204	641.342	-31.028	522.063	635.606	-166.000
250	317.413	548.602	616.517	-16.979	515.472	664.754	-138.890
298.15	387.605	610.530	610.530	0.000	509.619	694.051	-121.592
300	390.265	612.936	610.537	0.720	509.402	695.194	-121.041
350	460.150	678.398	615.547	21.998	504.016	726.598	-108.437
400	524.933	744.136	627.514	46.649	499.348	758.711	-99.075
450	583.633	809.415	644.105	74.389	495.304	791.379	-91.859
500	636.108	873.676	663.860	104.908	491.791	824.493	-86.132
600	724.033	997.745	709.260	173.091	486.046	891.602	-77.619
700	793.364	1114.769	758.918	249.095	481.810	959.557	-71.602
800	848.718	1224.455	810.330	331.300	478.918	1028.007	-67.121
900	893.593	1327.100	862.110	418.491	477.198	1096.740	-63.652
1000	930.471	1423.219	913.467	509.752	476.491	1165.624	-60.885
1100	961.118	1513.384	963.949	604.378	476.597	1234.550	-58.623
1200	986.823	1598.146	1013.303	701.812	477.374	1303.414	-56.735
1300	1008.550	1678.016	1061.392	801.610	478.637	1372.205	-55.135
1400	1027.042	1753.452	1108.156	903.414	480.249	1440.890	-53.759
1500	1042.878	1824.864	1153.578	1006.930	482.133	1509.452	-52.563
1600	1056.518	1892.616	1197.669	1111.917	484.151	1577.872	-51.511
1700	1068.331	1957.030	1240.458	1218.173	486.232	1646.138	-50.579
1800	1078.613	2018.392	1281.986	1325.532	488.295	1714.354	-49.748
1900	1087.607	2076.956	1322.297	1433.853	490.311	1782.395	-49.000
2000	1095.510	2132.948	1361.440	1543.017	492.228	1850.363	-48.326
2100	1102.484	2186.571	1399.464	1652.924	493.958	1918.224	-47.712
2200	1108.666	2238.004	1436.418	1763.487	495.506	1986.007	-47.153
2300	1114.165	2287.409	1472.351	1874.634	496.869	2053.726	-46.641
2400	1119.077	2334.934	1507.308	1986.301	497.968	2121.333	-46.169
2500	1123.479	2380.707	1541.334	2098.433	498.819	2189.031	-45.736
2600	1127.438	2424.850	1574.472	2210.982	499.385	2256.565	-45.334
2700	1131.009	2467.468	1606.761	2323.907	499.670	2324.169	-44.963
2800	1134.241	2508.659	1638.240	2437.172	499.647	2391.789	-44.618
2900	1137.175	2548.513	1668.946	2550.746	499.284	2459.356	-44.297
3000	1139.844	2587.111	1698.911	2664.599	498.633	2526.973	-43.998
3100	1142.279	2624.526	1728.169	2778.707	497.605	2594.525	-43.717
3200	1144.507	2660.828	1756.751	2893.048	496.250	2662.203	-43.455
3300	1146.550	2696.078	1784.684	3007.602	494.549	2729.975	-43.211
3400	1148.427	2730.334	1811.995	3122.352	492.467	2797.700	-42.981
3500	1150.156	2763.650	1838.712	3237.282	490.013	2865.472	-42.764
3600	1151.751	2796.073	1864.857	3352.379	487.213	2933.424	-42.562
3700	1153.226	2827.650	1890.453	3467.628	484.031	3001.473	-42.372
3800	1154.592	2858.423	1915.523	3583.020	480.439	3069.550	-42.193
3900	1155.860	2888.431	1940.086	3698.544	476.482	3137.660	-42.023
4000	1157.039	2917.710	1964.162	3814.189	472.144	3206.041	-41.866
4100	1158.137	2946.294	1987.770	3929.949	467.383	3274.450	-41.716
4200	1159.160	2974.214	2010.925	4045.814	462.233	3342.969	-41.575
4300	1160.117	3001.501	2033.646	4161.778	456.677	3411.511	-41.441
4400	1161.011	3028.182	2055.947	4277.835	450.726	3480.293	-41.315
4500	1161.849	3054.283	2077.843	4393.979	444.398	3549.277	-41.198
4600	1162.635	3079.828	2099.349	4510.203	437.630	3618.421	-41.088
4700	1163.373	3104.840	2120.477	4626.504	430.443	3687.582	-40.982
4800	1164.067	3129.340	2141.241	4742.876	422.887	3757.025	-40.884
4900	1164.720	3153.349	2161.652	4859.316	414.879	3826.470	-40.790
5000	1165.336	3176.886	2181.722	4975.819	406.526	3896.298	-40.704

3.553. Dibenzo[*de,ij*]naphtho[3,2,1,8,7-*rstuv*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-92-9
Point Group: C_s

Length: 15.69 Å
Width: 11.14 Å
Breadth: 3.888 Å
L/B Ratio: 1.408

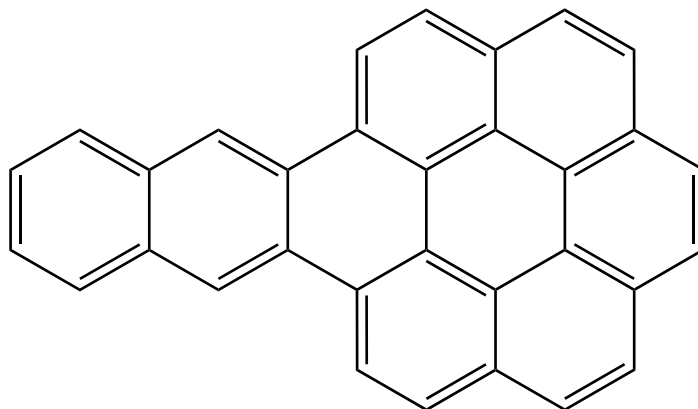
Cartesian coordinates:

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C	4.5418	2.7548	0.0000	C	1.1422	-1.0499	0.0000	H	5.0432	3.7283	0.0000
C	3.1409	2.7064	0.0000	C	-1.1731	2.5108	0.0000	H	2.5572	3.6399	0.0000
C	4.6323	0.3408	0.0000	C	-1.9427	3.6935	0.0000	H	5.3238	-3.0191	0.0000
C	4.7510	-2.0847	0.0000	C	-3.3180	3.6228	0.0000	H	6.4752	-0.8189	0.0000
C	5.3808	-0.8806	0.0000	C	-3.9645	2.3805	0.0000	H	0.7832	-4.4593	0.0000
C	3.3224	-2.1623	0.0000	C	-1.8188	1.2570	0.0000	H	3.2631	-4.3356	0.0000
C	1.2953	-3.4902	0.0000	C	-3.2371	1.1991	0.0000	H	-1.4024	-3.3502	0.0000
C	2.6571	-3.4223	0.0000	C	-1.6739	-1.2195	0.0000	H	0.7474	3.5535	0.0000
C	0.5060	-2.3021	0.0000	C	-1.0342	0.0599	0.0000	H	-1.4345	4.6643	0.0000
C	-0.9088	-2.3649	0.0000	C	-3.1327	-1.2824	0.0000	H	-3.9176	4.5391	0.0000
C	0.2520	2.5687	0.0000	C	-3.8960	-0.1021	0.0000	H	-5.0644	2.3344	0.0000
C	2.5695	-0.9851	0.0000	C	-5.2966	-0.1906	0.0000	H	-5.8851	0.7398	0.0000
C	3.2249	0.2888	0.0000	C	-5.9305	-1.4204	0.0000	H	-7.0239	-1.4749	0.0000
C	2.4716	1.4921	0.0000	C	-5.1736	-2.5925	0.0000	H	-5.6736	-3.5664	0.0000
C	1.0111	1.4289	0.0000	C	-3.7919	-2.5217	0.0000	H	-3.1888	-3.4428	0.0000

Table 3.553: Table of thermodynamic data as a function of temperature for Dibenzo[de,ij]naphtho[3,2,1,8,7-rstuv]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.539	474.629	474.629	∞
100	117.238	362.547	847.372	-48.483	501.603	548.976	-286.750
200	242.806	480.343	634.196	-30.771	487.331	602.046	-157.235
250	314.747	542.202	609.574	-16.843	480.619	631.500	-131.942
298.15	384.664	603.634	603.634	0.000	474.629	661.118	-115.823
300	387.317	606.021	603.641	0.714	474.408	662.273	-115.310
350	457.119	671.021	608.615	21.842	468.872	694.035	-103.577
400	521.953	736.356	620.500	46.343	464.052	726.527	-94.873
450	580.780	801.291	636.987	73.937	459.862	759.593	-88.169
500	633.421	865.260	656.626	104.317	456.211	793.121	-82.855
600	721.702	988.871	701.788	172.250	450.215	861.096	-74.963
700	791.359	1105.560	751.221	248.037	445.763	929.955	-69.393
800	846.987	1214.997	802.428	330.055	442.685	999.340	-65.249
900	892.088	1317.451	854.024	417.085	440.802	1069.028	-62.043
1000	929.152	1413.422	905.217	508.206	439.955	1138.885	-59.488
1100	959.955	1503.469	955.553	602.707	439.937	1208.796	-57.400
1200	985.790	1588.135	1004.776	700.031	440.605	1278.657	-55.657
1300	1007.627	1667.927	1052.748	799.732	441.769	1348.453	-54.180
1400	1026.214	1743.298	1099.407	901.449	443.294	1418.150	-52.911
1500	1042.131	1814.657	1144.733	1004.886	445.099	1487.730	-51.806
1600	1055.842	1882.363	1188.737	1109.801	447.047	1557.174	-50.835
1700	1067.716	1946.737	1231.447	1215.993	449.063	1626.467	-49.974
1800	1078.052	2008.066	1272.903	1323.293	451.067	1695.713	-49.207
1900	1087.094	2066.601	1313.148	1431.561	453.030	1764.789	-48.516
2000	1095.038	2122.568	1352.230	1540.676	454.897	1833.794	-47.893
2100	1102.050	2176.168	1390.198	1650.537	456.583	1902.693	-47.326
2200	1108.265	2227.582	1427.100	1761.059	458.089	1971.518	-46.809
2300	1113.794	2276.970	1462.984	1872.167	459.413	2040.281	-46.335
2400	1118.733	2324.479	1497.896	1983.798	460.476	2108.932	-45.899
2500	1123.159	2370.239	1531.881	2095.897	461.294	2177.676	-45.499
2600	1127.139	2414.369	1564.979	2208.415	461.829	2246.257	-45.127
2700	1130.730	2456.976	1597.231	2321.312	462.085	2314.910	-44.784
2800	1133.980	2498.158	1628.676	2434.550	462.035	2383.580	-44.465
2900	1136.929	2538.003	1659.349	2548.098	461.647	2452.198	-44.168
3000	1139.613	2576.593	1689.284	2661.927	460.972	2520.866	-43.891
3100	1142.062	2614.001	1718.513	2776.012	459.922	2589.470	-43.631
3200	1144.302	2650.296	1747.067	2890.332	458.546	2658.200	-43.390
3300	1146.356	2685.540	1774.974	3004.867	456.824	2727.026	-43.164
3400	1148.244	2719.791	1802.262	3119.598	454.724	2795.805	-42.951
3500	1149.982	2753.101	1828.955	3234.511	452.252	2864.632	-42.751
3600	1151.586	2785.520	1855.078	3349.590	449.436	2933.639	-42.565
3700	1153.070	2817.092	1880.653	3464.824	446.237	3002.744	-42.390
3800	1154.444	2847.861	1905.703	3580.200	442.630	3071.876	-42.225
3900	1155.719	2877.865	1930.247	3695.709	438.659	3141.043	-42.069
4000	1156.904	2907.140	1954.305	3811.341	434.307	3210.481	-41.924
4100	1158.008	2935.721	1977.895	3927.087	429.533	3279.947	-41.786
4200	1159.038	2963.639	2001.034	4042.940	424.370	3349.524	-41.657
4300	1159.999	2990.923	2023.739	4158.893	418.802	3419.123	-41.533
4400	1160.899	3017.601	2046.024	4274.938	412.840	3488.962	-41.418
4500	1161.741	3043.699	2067.906	4391.071	406.500	3559.005	-41.311
4600	1162.532	3069.242	2089.397	4507.285	399.722	3629.207	-41.210
4700	1163.274	3094.252	2110.512	4623.575	392.525	3699.428	-41.114
4800	1163.972	3118.750	2131.263	4739.938	384.959	3769.929	-41.024
4900	1164.629	3142.757	2151.661	4856.368	376.942	3840.433	-40.939
5000	1165.248	3166.292	2171.719	4972.862	368.580	3911.320	-40.860

3.554. Naphtho[2,3-*a*]coronene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 190-74-9
Point Group: C_{2v}

Length: 16.54 Å
Width: 11.65 Å
Breadth: 3.890 Å
L/B Ratio: 1.420

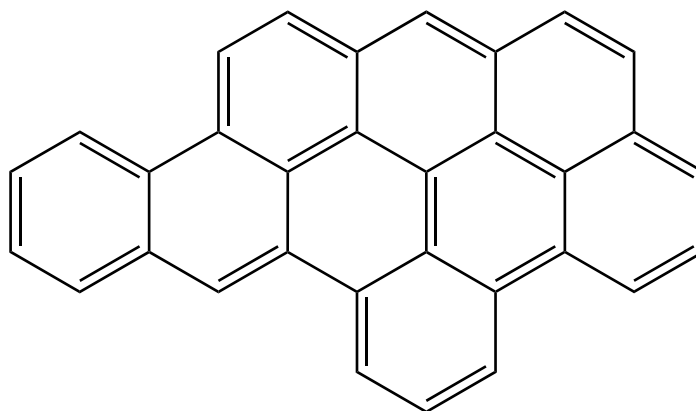
Cartesian coordinates:

C	-0.6964	2.8495	0.0000	C	1.6949	-1.4316	0.0000	H	-1.6520	3.3963	0.0000
C	0.4943	3.5298	0.0000	C	1.7027	-2.8367	0.0000	H	0.5086	4.6257	0.0000
C	1.7211	2.8256	0.0000	C	2.9527	-3.5332	0.0000	H	5.1096	3.3554	0.0000
C	1.7041	1.4206	0.0000	C	4.1309	-2.8539	0.0000	H	2.9667	4.6101	0.0000
C	4.1494	2.8270	0.0000	C	4.1508	-1.4237	0.0000	H	6.3163	-1.2616	0.0000
C	2.9756	3.5140	0.0000	C	2.9382	-0.7217	0.0000	H	6.3243	1.2207	0.0000
C	4.1599	1.3967	0.0000	C	-2.0060	-0.7066	0.0000	H	-1.6740	-3.3855	0.0000
C	2.9428	0.7026	0.0000	C	-2.0014	0.7195	0.0000	H	0.4787	-4.6289	0.0000
C	5.3742	-0.7014	0.0000	C	-3.2065	1.4056	0.0000	H	2.9368	-4.6292	0.0000
C	5.3786	0.6666	0.0000	C	-3.2156	-1.3847	0.0000	H	5.0877	-3.3885	0.0000
C	0.4656	0.7205	0.0000	C	-4.4402	-0.6924	0.0000	H	-3.2010	2.5076	0.0000
C	-0.7347	1.4343	0.0000	C	-4.4356	0.7212	0.0000	H	-3.2172	-2.4867	0.0000
C	0.4609	-0.7235	0.0000	C	-5.6790	1.4213	0.0000	H	-5.6661	2.5170	0.0000
C	-0.7440	-1.4295	0.0000	C	-6.8566	0.7322	0.0000	H	-7.8141	1.2635	0.0000
C	-0.7148	-2.8449	0.0000	C	-6.8612	-0.6877	0.0000	H	-7.8221	-1.2127	0.0000
C	0.4715	-3.5330	0.0000	C	-5.6882	-1.3844	0.0000	H	-5.6823	-2.4801	0.0000

Table 3.554: Table of thermodynamic data as a function of temperature for Naphtho[2,3-*a*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	
0	0.0	0.0	∞	-55.305	456.962	456.962	∞
100	115.702	353.645	837.284	-48.364	484.054	532.317	-278.048
200	242.286	470.607	624.437	-30.766	469.668	586.330	-153.131
250	314.745	532.411	599.812	-16.850	462.943	616.273	-128.760
298.15	384.944	593.869	593.869	0.000	456.962	646.362	-113.238
300	387.604	596.258	593.876	0.715	456.740	647.535	-112.744
350	457.527	661.313	598.854	21.861	451.222	679.783	-101.450
400	522.389	726.705	610.749	46.382	446.424	712.760	-93.075
450	581.202	791.690	627.250	73.998	442.256	746.307	-86.627
500	633.815	855.703	646.905	104.399	438.625	780.313	-81.517
600	722.040	979.380	692.100	172.368	432.666	849.241	-73.931
700	791.663	1096.119	741.565	248.187	428.245	919.047	-68.579
800	847.272	1205.595	792.802	330.235	425.196	989.373	-64.598
900	892.362	1308.082	844.424	417.292	423.342	1060.000	-61.520
1000	929.418	1404.081	895.641	508.440	422.522	1130.792	-59.065
1100	960.212	1494.153	946.000	602.968	422.530	1201.637	-57.060
1200	986.038	1578.841	995.244	700.317	423.223	1272.428	-55.386
1300	1007.865	1658.652	1043.235	800.042	424.412	1343.153	-53.967
1400	1026.439	1734.041	1089.911	901.782	425.960	1413.776	-52.748
1500	1042.345	1805.414	1135.254	1005.241	427.787	1484.281	-51.686
1600	1056.044	1873.134	1179.273	1110.178	429.755	1554.648	-50.753
1700	1067.906	1937.521	1221.998	1216.389	431.791	1624.863	-49.925
1800	1078.231	1998.859	1263.466	1323.708	433.813	1695.031	-49.188
1900	1087.261	2057.404	1303.724	1431.992	435.794	1765.027	-48.523
2000	1095.196	2113.379	1342.817	1541.123	437.677	1834.951	-47.923
2100	1102.198	2166.987	1380.796	1651.000	439.378	1904.769	-47.378
2200	1108.404	2218.407	1417.709	1761.536	440.898	1974.512	-46.880
2300	1113.925	2267.802	1453.602	1872.658	442.236	2044.191	-46.424
2400	1118.855	2315.316	1488.524	1984.302	443.312	2113.760	-46.004
2500	1123.274	2361.081	1522.516	2096.412	444.142	2183.419	-45.619
2600	1127.248	2405.215	1555.622	2208.942	444.688	2252.916	-45.261
2700	1130.833	2447.827	1587.883	2321.849	444.955	2322.485	-44.930
2800	1134.077	2489.012	1619.334	2435.097	444.915	2392.069	-44.624
2900	1137.021	2528.860	1650.014	2548.654	444.536	2461.601	-44.337
3000	1139.700	2567.453	1679.955	2662.492	443.870	2531.183	-44.071
3100	1142.145	2604.864	1709.191	2776.587	442.828	2600.701	-43.821
3200	1144.381	2641.161	1737.751	2890.914	441.460	2670.345	-43.588
3300	1146.431	2676.408	1765.663	3005.456	439.746	2740.085	-43.371
3400	1148.314	2710.660	1792.956	3120.195	437.653	2809.777	-43.166
3500	1150.049	2743.973	1819.654	3235.114	435.188	2879.516	-42.974
3600	1151.650	2776.393	1845.782	3350.200	432.378	2949.436	-42.794
3700	1153.130	2807.968	1871.362	3465.440	429.186	3019.453	-42.626
3800	1154.502	2838.738	1896.416	3580.823	425.585	3089.498	-42.467
3900	1155.774	2868.744	1920.965	3696.337	421.619	3159.577	-42.317
4000	1156.957	2898.020	1945.027	3811.975	417.273	3229.927	-42.178
4100	1158.059	2926.602	1968.620	3927.726	412.504	3300.305	-42.046
4200	1159.086	2954.521	1991.763	4043.584	407.346	3370.794	-41.921
4300	1160.046	2981.806	2014.471	4159.541	401.783	3441.305	-41.803
4400	1160.943	3008.486	2036.760	4275.591	395.825	3512.056	-41.693
4500	1161.784	3034.585	2058.645	4391.728	389.490	3583.009	-41.590
4600	1162.573	3060.128	2080.140	4507.946	382.716	3654.124	-41.493
4700	1163.313	3085.139	2101.258	4624.241	375.523	3725.255	-41.401
4800	1164.010	3109.638	2122.012	4740.607	367.961	3796.668	-41.315
4900	1164.665	3133.646	2142.413	4857.041	359.947	3868.083	-41.233
5000	1165.283	3157.182	2162.474	4973.539	351.589	3939.881	-41.159

3.555. Anthra[2,1,9,8,7-*defghi*]benzo[*st*]pentacene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-08-0
Point Group: C_s

Length: 16.57 Å
Width: 11.67 Å
Breadth: 3.885 Å
L/B Ratio: 1.420

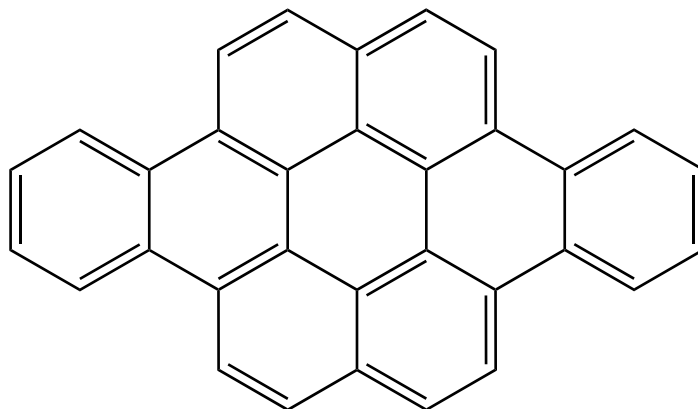
Cartesian coordinates:

C	-2.9033	-1.6717	0.0000	C	-4.1077	-0.9190	0.0000	H	-2.9601	-2.7725	0.0000
C	-2.7780	1.1402	0.0000	C	-4.0550	0.4886	0.0000	H	-1.4182	4.2920	0.0000
C	-1.4826	3.1979	0.0000	C	-5.2709	1.2197	0.0000	H	-3.6259	3.1418	0.0000
C	-2.6848	2.5703	0.0000	C	-6.4773	0.5703	0.0000	H	1.0220	4.1849	0.0000
C	-0.2638	2.4430	0.0000	C	-6.5271	-0.8405	0.0000	H	-1.4459	-3.7358	0.0000
C	0.9817	3.0886	0.0000	C	-5.3685	-1.5718	0.0000	H	0.6637	-5.0572	0.0000
C	2.0022	-1.9189	0.0000	C	3.2884	-1.2384	0.0000	H	2.8700	-3.8959	0.0000
C	-0.4711	-3.2242	0.0000	C	4.4906	-1.9491	0.0000	H	-5.2169	2.3190	0.0000
C	0.7072	-3.9631	0.0000	C	5.7112	-1.2824	0.0000	H	-7.4133	1.1385	0.0000
C	1.9328	-3.3183	0.0000	C	5.7556	0.1040	0.0000	H	-7.5009	-1.3410	0.0000
C	-0.4379	-1.8290	0.0000	C	3.3257	0.1736	0.0000	H	-5.3979	-2.6673	0.0000
C	0.8097	-1.1668	0.0000	C	4.5677	0.8443	0.0000	H	4.4578	-3.0495	0.0000
C	0.8645	0.2761	0.0000	C	4.5915	2.2864	0.0000	H	6.6425	-1.8584	0.0000
C	-0.3296	1.0320	0.0000	C	3.4465	3.0026	0.0000	H	6.7197	0.6250	0.0000
C	-1.6063	0.3773	0.0000	C	2.1591	2.3505	0.0000	H	5.5687	2.7830	0.0000
C	-1.6759	-1.0541	0.0000	C	2.1048	0.9325	0.0000	H	3.4656	4.0986	0.0000

Table 3.555: Table of thermodynamic data as a function of temperature for Anthra[2,1,9,8,7-defghi]benzo[st]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.634	476.097	476.097	∞
100	117.435	362.115	847.886	-48.577	502.976	550.393	-287.490
200	243.322	480.155	634.295	-30.828	488.741	603.494	-157.613
250	315.343	542.139	609.628	-16.872	482.057	632.954	-132.246
298.15	385.285	603.678	603.678	0.000	476.097	662.573	-116.078
300	387.939	606.070	603.685	0.715	475.877	663.728	-115.563
350	457.728	671.164	608.667	21.874	470.372	695.484	-103.793
400	522.527	736.579	620.568	46.404	465.582	727.968	-95.061
450	581.309	801.579	637.076	74.026	461.420	761.021	-88.335
500	633.901	865.601	656.738	104.432	457.793	794.533	-83.003
600	722.090	989.291	701.945	172.407	451.841	862.469	-75.083
700	791.672	1106.034	751.420	248.230	447.423	931.284	-69.492
800	847.240	1215.509	802.664	330.276	444.373	1000.619	-65.332
900	892.294	1317.990	854.292	417.329	442.514	1070.255	-62.115
1000	929.323	1413.981	905.513	508.468	441.686	1140.057	-59.549
1100	960.098	1504.042	955.874	602.985	441.683	1209.912	-57.453
1200	985.910	1588.720	1005.118	700.323	442.364	1279.714	-55.703
1300	1007.731	1668.521	1053.110	800.035	443.540	1349.452	-54.221
1400	1026.303	1743.899	1099.785	901.761	445.074	1419.088	-52.946
1500	1042.209	1815.263	1145.126	1005.206	446.888	1488.609	-51.837
1600	1055.910	1882.974	1189.144	1110.129	448.842	1557.991	-50.862
1700	1067.776	1947.353	1231.866	1216.327	450.865	1627.223	-49.997
1800	1078.106	2008.684	1273.333	1323.633	452.875	1696.408	-49.227
1900	1087.141	2067.222	1313.587	1431.905	454.843	1765.421	-48.534
2000	1095.081	2123.191	1352.679	1541.025	456.714	1834.364	-47.908
2100	1102.089	2176.793	1390.655	1650.890	458.404	1903.201	-47.339
2200	1108.300	2228.209	1427.565	1761.416	459.914	1971.963	-46.819
2300	1113.826	2277.599	1463.456	1872.528	461.241	2040.663	-46.344
2400	1118.762	2325.109	1498.375	1984.162	462.307	2109.252	-45.906
2500	1123.186	2370.871	1532.365	2096.263	463.128	2177.932	-45.504
2600	1127.164	2415.002	1565.469	2208.784	463.665	2246.450	-45.131
2700	1130.753	2457.610	1597.727	2321.683	463.924	2315.040	-44.786
2800	1134.001	2498.792	1629.177	2434.923	463.877	2383.646	-44.467
2900	1136.949	2538.638	1659.854	2548.473	463.491	2452.201	-44.168
3000	1139.632	2577.228	1689.793	2662.304	462.818	2520.805	-43.890
3100	1142.080	2614.637	1719.027	2776.392	461.769	2589.346	-43.629
3200	1144.319	2650.932	1747.585	2890.713	460.395	2658.013	-43.387
3300	1146.372	2686.177	1775.495	3005.249	458.675	2726.775	-43.160
3400	1148.258	2720.428	1802.786	3119.982	456.575	2795.490	-42.947
3500	1149.996	2753.738	1829.483	3234.896	454.105	2864.253	-42.746
3600	1151.599	2786.158	1855.609	3349.977	451.290	2933.196	-42.559
3700	1153.082	2817.731	1881.187	3465.212	448.093	3002.237	-42.383
3800	1154.455	2848.500	1906.240	3580.589	444.487	3071.306	-42.217
3900	1155.730	2878.504	1930.786	3696.099	440.517	3140.409	-42.060
4000	1156.915	2907.780	1954.847	3811.732	436.166	3209.783	-41.915
4100	1158.018	2936.361	1978.439	3927.480	431.393	3279.185	-41.776
4200	1159.047	2964.279	2001.580	4043.333	426.231	3348.698	-41.646
4300	1160.008	2991.563	2024.287	4159.287	420.664	3418.233	-41.522
4400	1160.907	3018.241	2046.575	4275.333	414.703	3488.008	-41.407
4500	1161.749	3044.340	2068.458	4391.466	408.364	3557.987	-41.299
4600	1162.539	3069.883	2089.952	4507.681	401.587	3628.125	-41.198
4700	1163.281	3094.892	2111.068	4623.973	394.390	3698.281	-41.101
4800	1163.979	3119.391	2131.821	4740.336	386.825	3768.719	-41.011
4900	1164.635	3143.398	2152.221	4856.767	378.808	3839.159	-40.925
5000	1165.255	3166.933	2172.281	4973.262	370.447	3909.982	-40.846

3.556. Dibenzo[*a,j*]coronene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 190-72-7
Point Group: D_{2h}

Length: 16.56 Å
Width: 11.66 Å
Breadth: 3.890 Å
L/B Ratio: 1.420

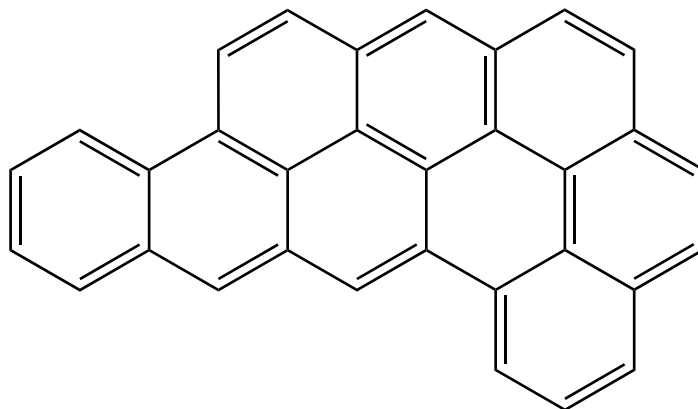
Cartesian coordinates:

C	-2.4111	2.8536	0.0000	C	1.2392	-0.7227	0.0000	H	-3.3709	3.3927	0.0000
C	-1.2280	3.5339	0.0000	C	2.4420	-1.4314	0.0000	H	-1.2127	4.6298	0.0000
C	0.0079	2.8312	0.0000	C	2.4500	1.4177	0.0000	H	3.3898	3.3738	0.0000
C	0.0040	1.4258	0.0000	C	1.2432	0.7157	0.0000	H	1.2385	4.6230	0.0000
C	2.4270	2.8400	0.0000	C	-3.7013	-0.6930	0.0000	H	-3.3899	-3.3738	0.0000
C	1.2478	3.5270	0.0000	C	-3.6974	0.7137	0.0000	H	-1.2386	-4.6230	0.0000
C	-1.2392	0.7227	0.0000	C	-4.9295	1.4037	0.0000	H	1.2126	-4.6299	0.0000
C	-2.4420	1.4314	0.0000	C	-6.1228	0.7190	0.0000	H	3.3709	-3.3928	0.0000
C	-1.2433	-0.7158	0.0000	C	-6.1267	-0.6846	0.0000	H	-4.9152	2.5044	0.0000
C	-2.4500	-1.4177	0.0000	C	-4.9374	-1.3760	0.0000	H	-7.0728	1.2632	0.0000
C	-2.4270	-2.8401	0.0000	C	3.7013	0.6931	0.0000	H	-7.0798	-1.2235	0.0000
C	-1.2478	-3.5271	0.0000	C	3.6974	-0.7138	0.0000	H	-4.9292	-2.4768	0.0000
C	-0.0040	-1.4259	0.0000	C	4.9296	-1.4037	0.0000	H	4.9154	-2.5043	0.0000
C	-0.0079	-2.8313	0.0000	C	6.1229	-0.7189	0.0000	H	7.0729	-1.2630	0.0000
C	1.2280	-3.5340	0.0000	C	6.1268	0.6848	0.0000	H	7.0798	1.2236	0.0000
C	2.4111	-2.8536	0.0000	C	4.9373	1.3761	0.0000	H	4.9291	2.4769	0.0000

Table 3.556: Table of thermodynamic data as a function of temperature for Dibenzo[*a,j*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-55.643	459.921	459.921	∞
100	117.864	350.809	836.123	-48.531	486.846	535.393	-279.655
200	243.046	468.900	622.795	-30.779	472.614	589.618	-153.989
250	314.826	530.796	598.169	-16.843	465.910	619.643	-129.465
298.15	384.608	592.229	592.229	0.000	459.921	649.810	-113.842
300	387.257	594.616	592.236	0.714	459.699	650.986	-113.344
350	456.955	659.598	597.209	21.836	454.157	683.318	-101.978
400	521.720	724.907	609.090	46.327	449.328	716.383	-93.548
450	580.505	789.811	625.571	73.908	445.125	750.022	-87.059
500	633.120	853.750	645.202	104.274	441.459	784.124	-81.915
600	721.373	977.303	690.345	172.175	435.432	853.253	-74.281
700	791.014	1093.940	739.757	247.928	430.946	923.272	-68.894
800	846.631	1203.330	790.941	329.911	427.832	993.821	-64.889
900	891.727	1305.742	842.514	416.905	425.914	1064.678	-61.791
1000	928.792	1401.675	893.686	507.990	425.031	1135.708	-59.322
1100	959.601	1491.688	944.001	602.456	424.977	1206.796	-57.305
1200	985.447	1576.324	993.203	699.745	425.610	1277.836	-55.622
1300	1007.298	1656.089	1041.156	799.412	426.741	1348.815	-54.195
1400	1025.900	1731.436	1087.796	901.096	428.234	1419.696	-52.968
1500	1041.834	1802.773	1133.105	1004.503	430.008	1490.464	-51.902
1600	1055.561	1870.461	1177.092	1109.390	431.927	1561.097	-50.964
1700	1067.452	1934.819	1219.787	1215.554	433.915	1631.581	-50.131
1800	1077.804	1996.133	1261.228	1322.829	435.894	1702.020	-49.390
1900	1086.860	2054.654	1301.459	1431.072	437.833	1772.290	-48.723
2000	1094.819	2110.610	1340.528	1540.164	439.677	1842.490	-48.120
2100	1101.844	2164.200	1378.483	1650.005	441.342	1912.586	-47.572
2200	1108.071	2215.604	1415.374	1760.507	442.828	1982.608	-47.072
2300	1113.612	2264.984	1451.247	1871.596	444.133	2052.568	-46.614
2400	1118.562	2312.486	1486.149	1983.209	445.178	2122.419	-46.192
2500	1122.998	2358.239	1520.123	2095.291	445.980	2192.362	-45.806
2600	1126.987	2402.363	1553.212	2207.794	446.499	2262.144	-45.446
2700	1130.587	2444.965	1585.455	2320.676	446.741	2331.998	-45.114
2800	1133.845	2486.141	1616.891	2433.900	446.677	2401.869	-44.806
2900	1136.802	2525.982	1647.556	2547.435	446.276	2471.689	-44.519
3000	1139.493	2564.567	1677.483	2661.251	445.589	2541.559	-44.252
3100	1141.948	2601.972	1706.705	2775.325	444.526	2611.366	-44.000
3200	1144.194	2638.263	1735.252	2889.634	443.139	2681.299	-43.767
3300	1146.254	2673.504	1763.153	3004.158	441.407	2751.329	-43.549
3400	1148.146	2707.751	1790.434	3118.879	439.296	2821.312	-43.343
3500	1149.889	2741.059	1817.121	3233.782	436.815	2891.342	-43.150
3600	1151.498	2773.475	1843.238	3348.853	433.990	2961.554	-42.970
3700	1152.985	2805.045	1868.808	3464.078	430.783	3031.863	-42.801
3800	1154.363	2835.812	1893.852	3579.446	427.167	3102.200	-42.642
3900	1155.642	2865.814	1918.391	3694.947	423.188	3172.572	-42.491
4000	1156.831	2895.087	1942.444	3810.571	418.828	3243.215	-42.351
4100	1157.938	2923.666	1966.030	3926.310	414.048	3313.886	-42.219
4200	1158.970	2951.582	1989.164	4042.156	408.878	3384.669	-42.094
4300	1159.935	2978.865	2011.864	4158.102	403.303	3455.474	-41.975
4400	1160.837	3005.542	2034.146	4274.141	397.334	3526.519	-41.864
4500	1161.682	3031.638	2056.023	4390.268	390.989	3597.768	-41.761
4600	1162.475	3057.180	2077.511	4506.476	384.205	3669.177	-41.664
4700	1163.219	3082.188	2098.622	4622.761	377.002	3740.603	-41.571
4800	1163.919	3106.685	2119.369	4739.118	369.431	3812.311	-41.486
4900	1164.578	3130.691	2139.764	4855.543	361.409	3884.022	-41.403
5000	1165.199	3154.225	2159.819	4972.033	353.042	3956.115	-41.328

3.557. Anthra[2,1,9,8,7-*defghi*]benzo[*uv*]pentacene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-13-7
Point Group: C_s

Length: 16.74 Å
Width: 11.36 Å
Breadth: 3.886 Å
L/B Ratio: 1.474

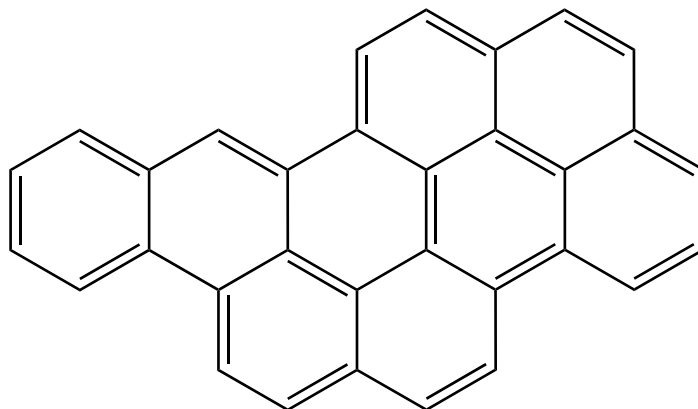
Cartesian coordinates:

C	0.5100	1.8254	0.0000	C	-0.5960	-0.3418	0.0000	H	0.4662	2.9270	0.0000
C	-0.4682	-3.1587	0.0000	C	-0.6468	1.1043	0.0000	H	-0.4243	-4.2549	0.0000
C	-1.7186	-2.5171	0.0000	C	1.7990	1.1891	0.0000	H	-5.0748	-3.2280	0.0000
C	-4.1441	-2.6490	0.0000	C	2.9657	1.9309	0.0000	H	-2.8690	-4.3661	0.0000
C	-2.9362	-3.2721	0.0000	C	3.1042	-0.8888	0.0000	H	-6.5529	1.2972	0.0000
C	-4.2313	-1.2214	0.0000	C	1.8649	-0.2371	0.0000	H	-6.4071	-1.1821	0.0000
C	-5.5802	0.7920	0.0000	C	0.6479	-0.9945	0.0000	H	-1.1503	3.7527	0.0000
C	-5.5004	-0.5662	0.0000	C	0.7051	-2.4165	0.0000	H	-3.3808	4.8547	0.0000
C	-4.3970	1.5959	0.0000	C	1.9953	-3.0561	0.0000	H	-5.4587	3.4886	0.0000
C	-2.0656	3.1408	0.0000	C	3.1348	-2.3269	0.0000	H	2.9231	3.0271	0.0000
C	-3.3245	3.7611	0.0000	C	4.2248	1.2906	0.0000	H	2.0276	-4.1517	0.0000
C	-4.4745	3.0068	0.0000	C	4.3044	-0.1205	0.0000	H	4.1242	-2.8100	0.0000
C	-1.9538	1.7603	0.0000	C	5.5882	-0.7349	0.0000	H	5.6335	-1.8348	0.0000
C	-3.1353	0.9701	0.0000	C	6.7259	0.0218	0.0000	H	7.7117	-0.4545	0.0000
C	-3.0628	-0.4598	0.0000	C	6.6443	1.4356	0.0000	H	7.5693	2.0215	0.0000
C	-1.7835	-1.1069	0.0000	C	5.4270	2.0559	0.0000	H	5.3546	3.1495	0.0000

Table 3.557: Table of thermodynamic data as a function of temperature for Anthra[2,1,9,8,7-defghi]benzo[uv]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.595	486.538	486.538	∞
100	116.759	361.493	847.353	-48.586	513.408	560.887	-292.971
200	243.415	479.232	633.612	-30.876	499.134	614.072	-160.376
250	315.866	541.287	608.902	-16.904	492.466	643.577	-134.465
298.15	386.043	602.941	602.941	0.000	486.538	673.234	-117.945
300	388.702	605.337	602.948	0.717	486.319	674.390	-117.419
350	458.586	670.558	607.939	21.917	480.855	706.180	-105.389
400	523.393	736.088	619.863	46.490	476.108	738.690	-96.461
450	582.142	801.188	636.401	74.154	471.989	771.766	-89.582
500	634.687	865.296	656.095	104.601	468.403	805.295	-84.127
600	722.779	989.121	701.371	172.650	462.524	873.255	-76.022
700	792.285	1105.964	750.911	248.537	458.172	942.081	-70.298
800	847.798	1215.517	802.215	330.642	455.180	1011.419	-66.038
900	892.810	1318.061	853.897	417.748	453.374	1081.051	-62.741
1000	929.802	1414.104	905.167	508.937	452.595	1150.843	-60.113
1100	960.545	1504.210	955.573	603.501	452.639	1220.683	-57.964
1200	986.328	1588.926	1004.858	700.881	453.363	1290.467	-56.171
1300	1008.120	1668.758	1052.887	800.633	454.580	1360.183	-54.652
1400	1026.665	1744.165	1099.596	902.397	456.151	1429.794	-53.345
1500	1042.546	1815.553	1144.968	1005.878	458.000	1499.287	-52.209
1600	1056.224	1883.285	1189.014	1110.833	459.987	1568.639	-51.210
1700	1068.068	1947.682	1231.763	1217.061	462.040	1637.838	-50.324
1800	1078.378	2009.029	1273.254	1324.395	464.078	1706.990	-49.535
1900	1087.395	2067.581	1313.532	1432.694	466.072	1775.968	-48.824
2000	1095.317	2123.563	1352.644	1541.838	467.968	1844.874	-48.182
2100	1102.310	2177.176	1390.640	1651.726	469.681	1913.674	-47.599
2200	1108.506	2228.602	1427.568	1762.273	471.212	1982.397	-47.067
2300	1114.019	2278.001	1463.477	1873.405	472.559	2051.057	-46.580
2400	1118.943	2325.519	1498.411	1985.058	473.644	2119.605	-46.131
2500	1123.355	2371.287	1532.417	2097.176	474.483	2188.244	-45.720
2600	1127.323	2415.425	1565.535	2209.714	475.036	2256.720	-45.337
2700	1130.903	2458.039	1597.806	2322.628	475.310	2325.268	-44.984
2800	1134.142	2499.226	1629.268	2435.883	475.277	2393.831	-44.657
2900	1137.082	2539.077	1659.958	2549.447	474.905	2462.341	-44.351
3000	1139.757	2577.672	1689.908	2663.291	474.245	2530.902	-44.066
3100	1142.198	2615.085	1719.152	2777.390	473.209	2599.398	-43.799
3200	1144.431	2651.384	1747.720	2891.723	471.846	2668.020	-43.550
3300	1146.478	2686.631	1775.640	3006.270	470.137	2736.737	-43.318
3400	1148.360	2720.886	1802.940	3121.014	468.048	2805.406	-43.099
3500	1150.092	2754.199	1829.646	3235.937	465.588	2874.123	-42.893
3600	1151.691	2786.621	1855.780	3351.027	462.782	2943.020	-42.701
3700	1153.169	2818.196	1881.366	3466.271	459.594	3012.015	-42.521
3800	1154.538	2848.968	1906.426	3581.658	455.996	3081.037	-42.351
3900	1155.809	2878.974	1930.980	3697.176	452.034	3150.093	-42.190
4000	1156.990	2908.252	1955.048	3812.816	447.691	3219.420	-42.040
4100	1158.090	2936.835	1978.646	3928.571	442.925	3288.774	-41.899
4200	1159.116	2964.754	2001.794	4044.432	437.770	3358.240	-41.765
4300	1160.074	2992.040	2024.507	4160.392	432.210	3427.728	-41.638
4400	1160.971	3018.720	2046.801	4276.445	426.255	3497.455	-41.519
4500	1161.810	3044.820	2068.690	4392.584	419.923	3567.385	-41.408
4600	1162.598	3070.364	2090.189	4508.805	413.151	3637.476	-41.304
4700	1163.337	3095.375	2111.311	4625.102	405.961	3707.584	-41.204
4800	1164.033	3119.875	2132.068	4741.471	398.401	3777.973	-41.112
4900	1164.687	3143.883	2152.473	4857.907	390.390	3848.365	-41.023
5000	1165.305	3167.419	2172.537	4974.407	382.034	3919.139	-40.942

3.558. Dinaphtho[2,1,8,7-*defg*:2',1',8',7'-*qrst*]pentacene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-94-1
Point Group: C_s

Length: 16.59 Å
Width: 11.13 Å
Breadth: 3.889 Å
L/B Ratio: 1.490

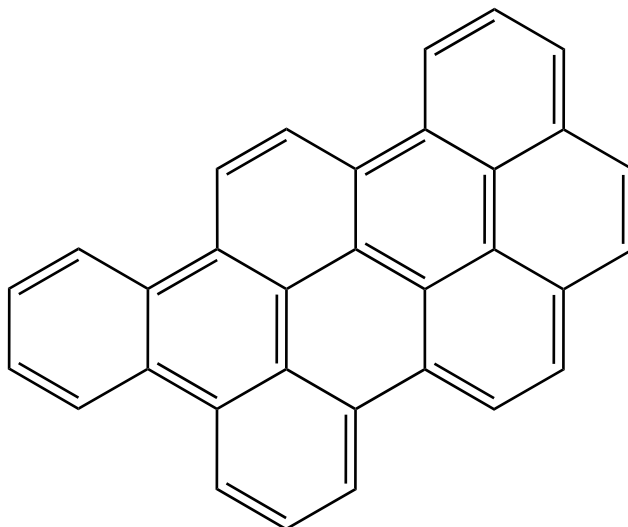
Cartesian coordinates:

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C	0.1532	-1.4704	0.0000	C	1.5129	-0.9407	0.0000	H	-1.5157	-4.4556	0.0000
C	-1.3554	-3.3714	0.0000	C	2.6045	-1.7733	0.0000	H	0.7937	-3.5343	0.0000
C	-0.0759	-2.8587	0.0000	C	1.7061	0.4810	0.0000	H	-5.8967	-2.5783	0.0000
C	-2.4654	-2.5089	0.0000	C	2.9995	1.0153	0.0000	H	-3.9435	-4.1112	0.0000
C	-4.8726	-2.1876	0.0000	C	3.1718	2.4345	0.0000	H	-4.1615	3.1000	0.0000
C	-3.8077	-3.0236	0.0000	C	2.1025	3.2733	0.0000	H	-6.4618	2.1534	0.0000
C	-4.6929	-0.7602	0.0000	C	0.7723	2.7524	0.0000	H	-6.8095	-0.3067	0.0000
C	-4.3116	2.0094	0.0000	C	0.5750	1.3601	0.0000	H	2.4580	-2.8657	0.0000
C	-5.5998	1.4781	0.0000	C	4.1357	0.1378	0.0000	H	4.2013	2.8248	0.0000
C	-5.7950	0.1077	0.0000	C	3.9281	-1.2550	0.0000	H	2.2402	4.3606	0.0000
C	-0.9411	-0.5952	0.0000	C	5.0461	-2.1288	0.0000	H	4.8736	-3.2110	0.0000
C	-0.7484	0.8365	0.0000	C	6.3204	-1.6235	0.0000	H	7.1848	-2.2956	0.0000
C	-1.8419	1.7059	0.0000	C	6.5314	-0.2286	0.0000	H	7.5557	0.1582	0.0000
C	-3.1957	1.1741	0.0000	C	5.4644	0.6323	0.0000	H	5.6143	1.7227	0.0000

Table 3.558: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1,8,7-*defg*:2',1',8',7'-*qrst*]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.938	467.225	467.225	∞
100	118.438	367.211	854.435	-48.722	493.959	540.865	-282.513
200	244.011	485.792	640.277	-30.897	479.800	593.425	-154.984
250	316.046	547.931	615.557	-16.907	473.150	622.600	-130.082
298.15	386.003	609.595	609.595	0.000	467.225	651.936	-114.214
300	388.657	611.991	609.603	0.717	467.005	653.080	-113.709
350	458.450	677.197	614.593	21.911	461.536	684.538	-102.160
400	523.242	742.708	626.514	46.478	456.782	716.717	-93.592
450	582.006	807.791	643.047	74.135	452.656	749.462	-86.993
500	634.572	871.885	662.736	104.575	449.063	782.661	-81.762
600	722.698	995.692	708.002	172.614	443.175	849.963	-73.994
700	792.211	1112.524	757.532	248.494	438.815	918.133	-68.511
800	847.716	1222.067	808.828	330.591	435.816	986.815	-64.431
900	892.714	1324.600	860.502	417.688	434.001	1055.793	-61.275
1000	929.694	1420.633	911.766	508.867	433.212	1124.931	-58.759
1100	960.427	1510.727	962.164	603.419	433.244	1194.119	-56.703
1200	986.203	1595.433	1011.443	700.788	433.957	1263.252	-54.987
1300	1007.993	1675.255	1059.465	800.527	435.160	1332.317	-53.532
1400	1026.538	1750.652	1106.168	902.278	436.719	1401.279	-52.281
1500	1042.421	1822.032	1151.534	1005.746	438.555	1470.124	-51.193
1600	1056.102	1889.756	1195.575	1110.689	440.530	1538.828	-50.237
1700	1067.951	1954.145	1238.318	1216.906	442.571	1607.381	-49.388
1800	1078.265	2015.486	1279.804	1324.228	444.597	1675.887	-48.632
1900	1087.287	2074.032	1320.077	1432.516	446.581	1744.220	-47.951
2000	1095.215	2130.009	1359.184	1541.649	448.466	1812.481	-47.336
2100	1102.212	2183.617	1397.175	1651.528	450.168	1880.636	-46.777
2200	1108.413	2235.038	1434.099	1762.065	451.690	1948.715	-46.267
2300	1113.931	2284.433	1470.004	1873.188	453.028	2016.732	-45.800
2400	1118.859	2331.947	1504.934	1984.832	454.104	2084.637	-45.370
2500	1123.276	2377.713	1538.936	2096.942	454.935	2152.633	-44.976
2600	1127.248	2421.847	1572.050	2209.472	455.481	2220.467	-44.609
2700	1130.832	2464.458	1604.318	2322.379	455.748	2288.372	-44.270
2800	1134.075	2505.643	1635.777	2435.627	455.708	2356.293	-43.956
2900	1137.018	2545.492	1666.463	2549.184	455.329	2424.163	-43.663
3000	1139.697	2584.084	1696.410	2663.022	454.663	2492.082	-43.390
3100	1142.141	2621.495	1725.652	2777.116	453.620	2559.936	-43.134
3200	1144.376	2657.793	1754.217	2891.443	452.252	2627.917	-42.895
3300	1146.426	2693.039	1782.134	3005.985	450.538	2695.994	-42.673
3400	1148.310	2727.291	1809.432	3120.723	448.444	2764.023	-42.463
3500	1150.045	2760.603	1836.134	3235.642	445.979	2832.099	-42.266
3600	1151.645	2793.024	1862.266	3350.727	443.168	2900.356	-42.082
3700	1153.126	2824.598	1887.850	3465.967	439.976	2968.710	-41.910
3800	1154.497	2855.369	1912.908	3581.349	436.374	3037.092	-41.747
3900	1155.769	2885.374	1937.460	3696.863	432.408	3105.508	-41.593
4000	1156.953	2914.650	1961.526	3812.500	428.061	3174.195	-41.450
4100	1158.054	2943.232	1985.122	3928.251	423.291	3242.909	-41.314
4200	1159.082	2971.151	2008.268	4044.108	418.133	3311.735	-41.187
4300	1160.041	2998.436	2030.979	4160.065	412.570	3380.584	-41.065
4400	1160.939	3025.115	2053.271	4276.114	406.611	3449.671	-40.952
4500	1161.780	3051.214	2075.159	4392.251	400.275	3518.962	-40.846
4600	1162.568	3076.758	2096.656	4508.468	393.501	3588.413	-40.747
4700	1163.309	3101.768	2117.776	4624.763	386.307	3657.882	-40.652
4800	1164.005	3126.267	2138.532	4741.129	378.746	3727.632	-40.564
4900	1164.661	3150.275	2158.936	4857.562	370.731	3797.384	-40.480
5000	1165.279	3173.811	2178.999	4974.060	362.372	3867.519	-40.403

3.559. Dibenzo[*ij,rst*]naphtho[2,1,8,7-*defg*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 75459-09-5
Point Group: C_s

Length: 15.93 Å
Width: 10.41 Å
Breadth: 3.886 Å
L/B Ratio: 1.531

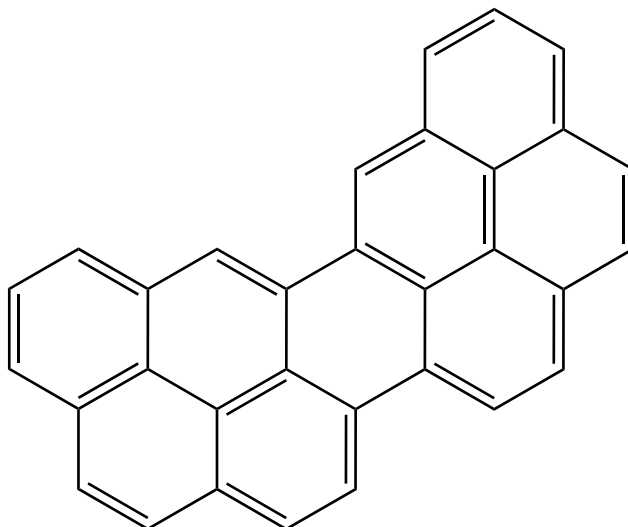
Cartesian coordinates:

C	3.6975	2.3759	0.0000	C	3.9089	-0.0971	0.0000	H	4.7959	2.4475	0.0000
C	2.9223	3.5267	0.0000	C	3.2899	-1.3582	0.0000	H	3.4042	4.5099	0.0000
C	1.5382	3.4339	0.0000	C	4.0901	-2.5152	0.0000	H	0.9207	4.3451	0.0000
C	3.0990	1.1119	0.0000	C	5.4677	-2.4241	0.0000	H	-0.6690	-3.7823	0.0000
C	1.8391	-1.4557	0.0000	C	6.0839	-1.1689	0.0000	H	1.8181	-3.6172	0.0000
C	-0.1754	-2.7980	0.0000	C	5.3135	-0.0231	0.0000	H	-0.8592	4.2240	0.0000
C	1.2011	-2.7054	0.0000	C	-2.4256	-1.7470	0.0000	H	-3.3391	4.0561	0.0000
C	-0.9731	-1.6445	0.0000	C	-5.2303	-1.9073	0.0000	H	3.5971	-3.4994	0.0000
C	-1.3521	3.2396	0.0000	C	-4.4638	-3.0578	0.0000	H	6.0797	-3.3318	0.0000
C	-2.7239	3.1490	0.0000	C	-3.0706	-2.9807	0.0000	H	7.1764	-1.0980	0.0000
C	1.0582	-0.2856	0.0000	C	-4.6097	-0.6470	0.0000	H	5.7912	0.9687	0.0000
C	1.6907	1.0108	0.0000	C	-3.2018	-0.5633	0.0000	H	-6.3244	-1.9700	0.0000
C	0.9068	2.1858	0.0000	C	-2.5671	0.7237	0.0000	H	-4.9487	-4.0397	0.0000
C	-0.5436	2.0832	0.0000	C	-3.3539	1.8882	0.0000	H	-2.4650	-3.9001	0.0000
C	-1.1509	0.8218	0.0000	C	-4.7857	1.7756	0.0000	H	-5.3770	2.6985	0.0000
C	-0.3543	-0.3816	0.0000	C	-5.3872	0.5618	0.0000	H	-6.4797	0.4735	0.0000

Table 3.559: Table of thermodynamic data as a function of temperature for Dibenzo[*ij,rst*]naphtho[2,1,8,7-*defg*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.738	465.340	465.340	∞
100	118.217	367.905	852.897	-48.499	492.297	539.134	-281.609
200	242.811	486.020	639.754	-30.747	478.065	591.645	-154.519
250	314.482	547.850	615.154	-16.826	471.346	620.816	-129.710
298.15	384.237	609.220	609.220	0.000	465.340	650.163	-113.904
300	386.885	611.605	609.227	0.713	465.117	651.308	-113.400
350	456.607	676.531	614.196	21.817	459.557	682.792	-101.899
400	521.417	741.796	626.067	46.291	454.711	715.011	-93.369
450	580.251	806.668	642.536	73.859	450.495	747.807	-86.801
500	632.911	870.582	662.155	104.213	446.817	781.066	-81.596
600	721.231	994.103	707.275	172.097	440.773	848.514	-73.868
700	790.914	1110.722	756.667	247.839	436.275	916.854	-68.415
800	846.557	1220.101	807.835	329.813	433.153	985.725	-64.360
900	891.668	1322.505	859.393	416.800	431.228	1054.906	-61.224
1000	928.743	1418.432	910.553	507.879	430.339	1124.259	-58.724
1100	959.558	1508.440	960.857	602.341	430.281	1193.672	-56.682
1200	985.408	1593.073	1010.051	699.626	430.910	1263.037	-54.977
1300	1007.263	1672.834	1057.996	799.289	432.037	1332.341	-53.533
1400	1025.868	1748.180	1104.629	900.970	433.526	1401.548	-52.291
1500	1041.804	1819.515	1149.932	1004.374	435.298	1470.642	-51.211
1600	1055.534	1887.200	1193.914	1109.258	437.214	1539.601	-50.262
1700	1067.426	1951.557	1236.604	1215.420	439.200	1608.411	-49.419
1800	1077.780	2012.869	1278.040	1322.692	441.176	1677.176	-48.669
1900	1086.838	2071.390	1318.267	1430.933	443.113	1745.772	-47.994
2000	1094.799	2127.344	1357.332	1540.023	444.955	1814.299	-47.384
2100	1101.825	2180.933	1395.285	1649.861	446.617	1882.722	-46.829
2200	1108.054	2232.336	1432.172	1760.361	448.101	1951.070	-46.323
2300	1113.596	2281.716	1468.042	1871.449	449.405	2019.358	-45.860
2400	1118.546	2329.217	1502.941	1983.061	450.449	2087.535	-45.433
2500	1122.983	2374.969	1536.913	2095.141	451.249	2155.805	-45.042
2600	1126.974	2419.093	1570.000	2207.643	451.767	2223.914	-44.678
2700	1130.574	2461.694	1602.241	2320.523	452.007	2292.095	-44.342
2800	1133.833	2502.870	1633.675	2433.746	451.942	2360.293	-44.031
2900	1136.790	2542.710	1664.338	2547.280	451.540	2428.440	-43.740
3000	1139.482	2581.295	1694.263	2661.095	450.851	2496.638	-43.469
3100	1141.938	2618.699	1723.484	2775.168	449.788	2564.772	-43.215
3200	1144.184	2654.990	1752.029	2889.476	448.400	2633.033	-42.979
3300	1146.244	2690.231	1779.928	3003.999	446.667	2701.389	-42.759
3400	1148.137	2724.478	1807.208	3118.719	444.555	2769.700	-42.550
3500	1149.881	2757.785	1833.893	3233.621	442.073	2838.057	-42.355
3600	1151.490	2790.201	1860.009	3348.691	439.247	2906.596	-42.173
3700	1152.978	2821.771	1885.578	3463.915	436.039	2975.233	-42.002
3800	1154.356	2852.538	1910.621	3579.283	432.423	3043.898	-41.840
3900	1155.635	2882.539	1935.159	3694.783	428.443	3112.597	-41.688
4000	1156.824	2911.813	1959.211	3810.407	424.083	3181.568	-41.546
4100	1157.932	2940.392	1982.795	3926.145	419.301	3250.566	-41.412
4200	1158.964	2968.307	2005.929	4041.991	414.131	3319.676	-41.285
4300	1159.929	2995.590	2028.628	4157.936	408.556	3388.809	-41.165
4400	1160.831	3022.267	2050.909	4273.974	402.586	3458.182	-41.053
4500	1161.677	3048.363	2072.785	4390.100	396.240	3527.757	-40.948
4600	1162.469	3073.904	2094.272	4506.308	389.456	3597.494	-40.850
4700	1163.214	3098.913	2115.382	4622.592	382.252	3667.248	-40.756
4800	1163.914	3123.410	2136.129	4738.949	374.681	3737.284	-40.669
4900	1164.573	3147.416	2156.523	4855.374	366.658	3807.321	-40.586
5000	1165.195	3170.950	2176.577	4971.863	358.291	3877.743	-40.510

3.560. Dinaphtho[2,1,8,7-*defg*:2',1',8',7'-*ijkl*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 188-90-9
Point Group: C_{2v}

Length: 15.94 Å
Width: 10.41 Å
Breadth: 3.885 Å
L/B Ratio: 1.532

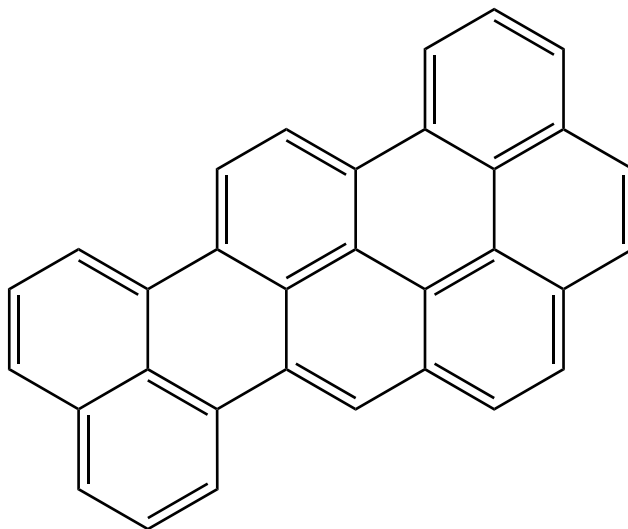
Cartesian coordinates:

C	0.7312	-0.6543	0.0000	C	-3.5696	-0.6089	0.0000	H	0.8999	-2.7862	0.0000
C	1.4357	-1.8229	0.0000	C	-2.8412	0.6243	0.0000	H	3.3761	4.0006	0.0000
C	0.7306	1.8349	0.0000	C	-3.5466	1.8475	0.0000	H	0.8929	3.9874	0.0000
C	1.4262	0.6143	0.0000	C	-4.9862	1.8309	0.0000	H	-0.9025	-2.7854	0.0000
C	2.8337	3.0483	0.0000	C	-5.6721	0.6646	0.0000	H	-0.8893	3.9882	0.0000
C	1.4504	3.0379	0.0000	C	-4.9827	-0.5999	0.0000	H	-3.3726	4.0036	0.0000
C	-0.7318	-0.6536	0.0000	C	2.8708	-1.8404	0.0000	H	-6.7727	-1.8118	0.0000
C	-1.4374	-1.8216	0.0000	C	3.5899	-3.0402	0.0000	H	-5.5362	-3.9624	0.0000
C	-1.4257	0.6156	0.0000	C	4.9794	-3.0222	0.0000	H	-3.0561	-3.9924	0.0000
C	-0.7290	1.8356	0.0000	C	5.6752	-1.8192	0.0000	H	-5.5107	2.7934	0.0000
C	-1.4477	3.0393	0.0000	C	3.5691	-0.6121	0.0000	H	-6.7681	0.6534	0.0000
C	-2.8309	3.0509	0.0000	C	4.9822	-0.6044	0.0000	H	3.0524	-3.9951	0.0000
C	-2.8724	-1.8377	0.0000	C	5.6728	0.6594	0.0000	H	5.5327	-3.9674	0.0000
C	-5.6768	-1.8140	0.0000	C	4.9879	1.8263	0.0000	H	6.7710	-1.8180	0.0000
C	-4.9822	-3.0177	0.0000	C	3.5483	1.8442	0.0000	H	6.7687	0.6472	0.0000
C	-3.5926	-3.0369	0.0000	C	2.8417	0.6217	0.0000	H	5.5132	2.7884	0.0000

Table 3.560: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1,8,7-*defg*:2',1',8',7'-*ijkl*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-55.394	485.879	485.879	∞
100	115.745	355.646	840.126	-48.448	512.887	560.950	-293.004
200	242.710	472.760	626.891	-30.826	498.525	614.757	-160.555
250	315.367	534.680	602.217	-16.884	491.827	644.589	-134.677
298.15	385.725	596.262	596.262	0.000	485.879	674.566	-118.179
300	388.391	598.656	596.269	0.716	485.659	675.734	-117.653
350	458.434	663.841	601.257	21.904	480.183	707.859	-105.640
400	523.367	729.360	613.176	46.474	475.433	740.706	-96.724
450	582.210	794.463	629.709	74.139	471.314	774.118	-89.855
500	634.820	858.581	649.400	104.590	467.733	807.983	-84.408
600	722.988	982.437	694.675	172.657	461.872	876.613	-76.314
700	792.520	1099.315	744.219	248.567	457.542	946.106	-70.598
800	848.037	1208.900	795.531	330.696	454.575	1016.107	-66.344
900	893.040	1311.472	847.222	417.825	452.792	1086.399	-63.052
1000	930.020	1407.539	898.502	509.037	452.036	1156.849	-60.426
1100	960.747	1497.664	948.918	603.621	452.100	1227.345	-58.281
1200	986.515	1582.397	998.213	701.021	452.844	1297.782	-56.490
1300	1008.292	1662.244	1046.251	800.792	454.079	1368.150	-54.972
1400	1026.823	1737.663	1092.969	902.572	455.667	1438.412	-53.667
1500	1042.691	1809.061	1138.350	1006.068	457.531	1508.554	-52.531
1600	1056.358	1876.802	1182.404	1111.037	459.532	1578.555	-51.533
1700	1068.191	1941.207	1225.161	1217.278	461.597	1648.403	-50.648
1800	1078.491	2002.561	1266.659	1324.624	463.647	1718.201	-49.860
1900	1087.499	2061.119	1306.944	1432.933	465.652	1787.826	-49.150
2000	1095.414	2117.106	1346.062	1542.087	467.558	1857.378	-48.509
2100	1102.399	2170.724	1384.064	1651.985	469.280	1926.823	-47.926
2200	1108.590	2222.153	1420.999	1762.541	470.820	1996.191	-47.395
2300	1114.097	2271.556	1456.912	1873.680	472.175	2065.496	-46.908
2400	1119.015	2319.077	1491.852	1985.341	473.267	2134.688	-46.459
2500	1123.423	2364.849	1525.862	2097.466	474.113	2203.971	-46.049
2600	1127.386	2408.989	1558.985	2210.010	474.673	2273.091	-45.666
2700	1130.962	2451.605	1591.260	2322.931	474.954	2342.282	-45.313
2800	1134.198	2492.795	1622.726	2436.191	474.926	2411.488	-44.986
2900	1137.134	2532.647	1653.420	2549.760	474.559	2480.642	-44.680
3000	1139.807	2571.244	1683.374	2663.609	473.904	2549.845	-44.396
3100	1142.245	2608.658	1712.621	2777.714	472.873	2618.984	-44.129
3200	1144.475	2644.959	1741.193	2892.052	471.514	2688.248	-43.880
3300	1146.520	2680.208	1769.116	3006.603	469.810	2757.608	-43.648
3400	1148.399	2714.463	1796.419	3121.350	467.725	2826.920	-43.429
3500	1150.129	2747.778	1823.127	3236.278	465.269	2896.279	-43.224
3600	1151.726	2780.201	1849.264	3351.371	462.466	2965.818	-43.032
3700	1153.203	2811.777	1874.853	3466.619	459.282	3035.455	-42.852
3800	1154.570	2842.549	1899.916	3582.008	455.687	3105.118	-42.682
3900	1155.840	2872.556	1924.472	3697.530	451.729	3174.816	-42.521
4000	1157.019	2901.835	1948.542	3813.173	447.388	3244.785	-42.372
4100	1158.118	2930.418	1972.143	3928.931	442.626	3314.781	-42.230
4200	1159.143	2958.339	1995.292	4044.794	437.473	3384.888	-42.096
4300	1160.100	2985.625	2018.007	4160.757	431.916	3455.018	-41.969
4400	1160.995	3012.306	2040.303	4276.812	425.963	3525.387	-41.851
4500	1161.834	3038.406	2062.194	4392.954	419.633	3595.958	-41.740
4600	1162.620	3063.951	2083.695	4509.177	412.864	3666.690	-41.636
4700	1163.359	3088.962	2104.818	4625.477	405.676	3737.439	-41.536
4800	1164.053	3113.462	2125.577	4741.848	398.119	3808.470	-41.444
4900	1164.707	3137.471	2145.984	4858.286	390.109	3879.503	-41.355
5000	1165.324	3161.007	2166.050	4974.788	381.755	3950.918	-41.274

3.561. Dibenzo[*kl,rst*]naphtho[2,1,8,7-*defg*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120864-22-4
Point Group: C_s

Length: 15.95 Å
Width: 10.40 Å
Breadth: 3.885 Å
L/B Ratio: 1.534

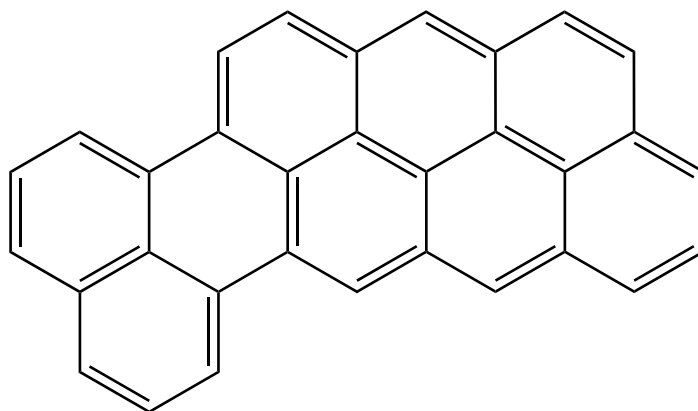
Cartesian coordinates:

C	0.9608	-2.6150	0.0000	C	-2.7678	0.8572	0.0000	H	1.5631	-3.5369	0.0000
C	-0.4290	-2.6945	0.0000	C	-3.4212	-0.4184	0.0000	H	-0.9282	-3.6760	0.0000
C	0.7124	2.2361	0.0000	C	-2.6632	-1.6166	0.0000	H	1.2017	3.2238	0.0000
C	-0.7135	2.1756	0.0000	C	0.8431	-0.1954	0.0000	H	-0.9877	4.3293	0.0000
C	-1.4967	3.3586	0.0000	C	1.6095	-1.3842	0.0000	H	-3.4675	4.2058	0.0000
C	-2.8645	3.2905	0.0000	C	1.4751	1.0999	0.0000	H	-5.5315	2.8843	0.0000
C	-3.5253	2.0360	0.0000	C	3.0685	-1.3093	0.0000	H	-6.6755	0.6808	0.0000
C	-4.9563	1.9513	0.0000	C	3.8454	-2.4499	0.0000	H	-6.5671	-1.7705	0.0000
C	-5.5814	0.7468	0.0000	C	5.2517	-2.3693	0.0000	H	-5.2260	-3.8632	0.0000
C	-4.8293	-0.4755	0.0000	C	5.8758	-1.1502	0.0000	H	-2.7389	-3.7662	0.0000
C	-5.4721	-1.7278	0.0000	C	2.9357	1.1751	0.0000	H	3.3575	-3.4368	0.0000
C	-4.7259	-2.8890	0.0000	C	3.6995	-0.0300	0.0000	H	5.8373	-3.2946	0.0000
C	-3.3286	-2.8365	0.0000	C	5.1090	0.0447	0.0000	H	6.9694	-1.0790	0.0000
C	-1.2071	-1.5421	0.0000	C	5.7454	1.3145	0.0000	H	6.8404	1.3591	0.0000
C	-0.5663	-0.2773	0.0000	C	4.9958	2.4600	0.0000	H	5.4795	3.4424	0.0000
C	-1.3466	0.9259	0.0000	C	3.5883	2.3909	0.0000	H	2.9992	3.3211	0.0000

Table 3.561: Table of thermodynamic data as a function of temperature for Dibenzo[*kl,rst*]naphtho[2,1,8,7-*defg*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-55.609	486.551	486.551	∞
100	117.183	365.794	850.736	-48.494	513.513	560.561	-292.801
200	242.869	483.522	637.478	-30.791	499.232	613.311	-160.177
250	314.973	545.414	612.838	-16.856	492.527	642.605	-134.262
298.15	384.973	606.894	606.894	0.000	486.551	672.068	-117.741
300	387.629	609.283	606.901	0.715	486.330	673.217	-117.215
350	457.466	674.334	611.879	21.859	480.810	704.814	-105.186
400	522.306	739.716	623.773	46.377	476.008	737.140	-96.259
450	581.127	804.692	640.272	73.989	471.836	770.037	-89.382
500	633.753	868.697	659.924	104.386	468.201	803.393	-83.928
600	721.998	992.365	705.115	172.350	462.237	871.021	-75.828
700	791.619	1109.097	754.575	248.166	457.813	939.529	-70.107
800	847.214	1218.567	805.807	330.208	454.759	1008.558	-65.851
900	892.287	1321.046	857.425	417.259	452.898	1077.888	-62.558
1000	929.328	1417.037	908.638	508.398	452.069	1147.385	-59.932
1100	960.110	1507.099	958.993	602.916	452.067	1216.934	-57.786
1200	985.928	1591.778	1008.232	700.255	452.750	1286.431	-55.996
1300	1007.751	1671.580	1056.220	799.969	453.928	1355.862	-54.478
1400	1026.325	1746.961	1102.891	901.697	455.464	1425.193	-53.174
1500	1042.232	1818.326	1148.229	1005.145	457.280	1494.407	-52.039
1600	1055.933	1886.038	1192.244	1110.070	459.237	1563.483	-51.041
1700	1067.799	1950.418	1234.965	1216.271	461.262	1632.408	-50.157
1800	1078.128	2011.751	1276.430	1323.579	463.274	1701.287	-49.369
1900	1087.163	2070.290	1316.683	1431.853	465.244	1769.993	-48.660
2000	1095.102	2126.260	1355.773	1540.975	467.118	1838.629	-48.019
2100	1102.109	2179.864	1393.748	1650.843	468.810	1907.159	-47.437
2200	1108.319	2231.280	1430.657	1761.370	470.321	1975.614	-46.906
2300	1113.844	2280.671	1466.547	1872.484	471.651	2044.007	-46.420
2400	1118.779	2328.182	1501.465	1984.119	472.718	2112.288	-45.972
2500	1123.202	2373.944	1535.455	2096.222	473.541	2180.662	-45.561
2600	1127.179	2418.075	1568.558	2208.745	474.080	2248.872	-45.179
2700	1130.768	2460.684	1600.815	2321.645	474.340	2317.155	-44.827
2800	1134.015	2501.867	1632.265	2434.887	474.294	2385.454	-44.500
2900	1136.962	2541.713	1662.942	2548.438	473.909	2453.701	-44.195
3000	1139.644	2580.304	1692.880	2662.271	473.238	2521.998	-43.911
3100	1142.091	2617.713	1722.114	2776.359	472.190	2590.230	-43.644
3200	1144.330	2654.009	1750.671	2890.682	470.817	2658.590	-43.396
3300	1146.382	2689.254	1778.581	3005.219	469.098	2727.044	-43.165
3400	1148.269	2723.505	1805.872	3119.953	467.000	2795.452	-42.946
3500	1150.006	2756.816	1832.568	3234.868	464.531	2863.907	-42.741
3600	1151.608	2789.235	1858.694	3349.949	461.716	2932.542	-42.549
3700	1153.091	2820.809	1884.272	3465.185	458.520	3001.276	-42.370
3800	1154.464	2851.578	1909.325	3580.564	454.915	3070.036	-42.200
3900	1155.738	2881.583	1933.871	3696.075	450.946	3138.831	-42.039
4000	1156.922	2910.858	1957.931	3811.709	446.596	3207.898	-41.890
4100	1158.025	2939.440	1981.523	3927.457	441.824	3276.991	-41.749
4200	1159.054	2967.358	2004.665	4043.311	436.662	3346.197	-41.615
4300	1160.015	2994.642	2027.371	4159.265	431.096	3415.424	-41.488
4400	1160.914	3021.321	2049.659	4275.312	425.135	3484.892	-41.370
4500	1161.756	3047.419	2071.542	4391.446	418.797	3554.562	-41.259
4600	1162.545	3072.962	2093.036	4507.661	412.021	3624.393	-41.155
4700	1163.287	3097.972	2114.152	4623.953	404.825	3694.241	-41.056
4800	1163.984	3122.471	2134.905	4740.317	397.260	3764.370	-40.964
4900	1164.641	3146.478	2155.305	4856.749	389.244	3834.502	-40.875
5000	1165.260	3170.013	2175.364	4973.244	380.883	3905.017	-40.795

3.562. Anthra[2,1,9,8,7-*defghi*]benzo[*op*]pentacene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120864-24-6
Point Group: C_s

Length: 16.74 Å
Width: 10.77 Å
Breadth: 3.885 Å
L/B Ratio: 1.554

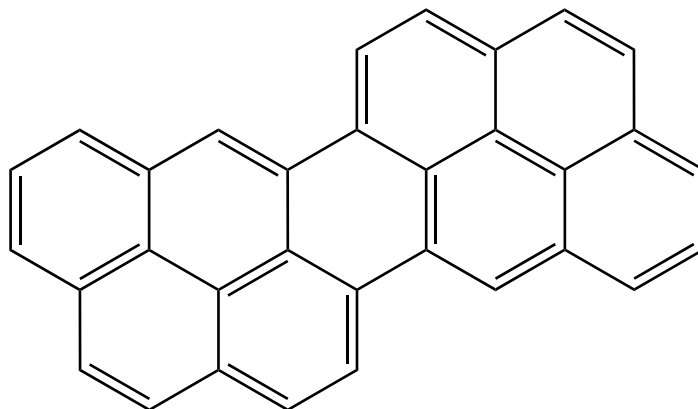
Cartesian coordinates:

C	0.2677	1.7817	0.0000	C	-5.1034	-0.0837	0.0000	H	0.4640	2.8665	0.0000
C	-1.1048	1.3391	0.0000	C	-5.3396	-1.5117	0.0000	H	-1.9611	3.3120	0.0000
C	-2.1512	2.2317	0.0000	C	-4.3187	-2.3925	0.0000	H	-4.3850	3.7535	0.0000
C	-3.4989	1.7735	0.0000	C	1.0681	-0.5257	0.0000	H	-6.7185	2.9113	0.0000
C	-4.5855	2.6762	0.0000	C	2.1166	-1.4439	0.0000	H	-7.1843	0.4776	0.0000
C	-5.8804	2.2063	0.0000	C	1.3088	0.9067	0.0000	H	0.3315	-4.3656	0.0000
C	-6.1464	0.8292	0.0000	C	3.5003	-0.9772	0.0000	H	2.6736	-3.5351	0.0000
C	0.5372	-3.2891	0.0000	C	4.5602	-1.8617	0.0000	H	-2.0811	-3.9207	0.0000
C	1.8294	-2.8281	0.0000	C	5.8901	-1.3992	0.0000	H	-6.3810	-1.8541	0.0000
C	-0.5464	-2.3804	0.0000	C	6.1571	-0.0555	0.0000	H	-4.5051	-3.4727	0.0000
C	-0.2761	-0.9940	0.0000	C	2.6936	1.3774	0.0000	H	4.3622	-2.9446	0.0000
C	-1.3607	-0.0715	0.0000	C	3.7576	0.4262	0.0000	H	6.7069	-2.1286	0.0000
C	-1.8922	-2.8401	0.0000	C	5.0930	0.8836	0.0000	H	7.1896	0.3118	0.0000
C	-2.9398	-1.9499	0.0000	C	5.3580	2.2794	0.0000	H	6.3992	2.6214	0.0000
C	-2.6795	-0.5408	0.0000	C	4.3243	3.1765	0.0000	H	4.5209	4.2537	0.0000
C	-3.7618	0.3856	0.0000	C	2.9890	2.7252	0.0000	H	2.1676	3.4584	0.0000

Table 3.562: Table of thermodynamic data as a function of temperature for Anthra[2,1,9,8,7-defghi]benzo[op]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.793	507.009	507.009	∞
100	117.189	365.726	852.776	-48.705	533.760	580.815	-303.380
200	244.055	483.825	638.533	-30.942	519.539	633.558	-165.465
250	316.544	546.029	613.774	-16.936	512.904	662.829	-138.488
298.15	386.709	607.801	607.801	0.000	507.009	692.255	-121.278
300	389.367	610.201	607.809	0.718	506.791	693.402	-120.730
350	459.216	675.523	612.808	21.950	501.359	724.946	-108.190
400	523.983	741.134	624.749	46.554	496.643	757.207	-98.879
450	582.690	806.302	641.308	74.247	492.552	790.028	-91.702
500	635.193	870.465	661.026	104.720	488.992	823.300	-86.008
600	723.209	994.375	706.349	172.816	483.160	890.739	-77.544
700	792.647	1111.279	755.933	248.742	478.847	959.036	-71.563
800	848.102	1220.877	807.276	330.880	475.889	1027.840	-67.110
900	893.066	1323.454	858.993	418.014	474.111	1096.935	-63.663
1000	930.020	1419.522	910.295	509.227	473.356	1166.186	-60.914
1100	960.730	1509.647	960.728	603.811	473.419	1235.483	-58.667
1200	986.487	1594.377	1010.037	701.208	474.161	1304.723	-56.792
1300	1008.257	1674.222	1058.087	800.976	475.392	1373.892	-55.203
1400	1026.785	1749.638	1104.815	902.752	476.977	1442.957	-53.836
1500	1042.651	1821.034	1150.204	1006.244	478.837	1511.902	-52.648
1600	1056.317	1888.772	1194.266	1111.209	480.834	1580.706	-51.604
1700	1068.151	1953.174	1237.029	1217.446	482.895	1649.356	-50.678
1800	1078.452	2014.526	1278.533	1324.788	484.941	1717.958	-49.853
1900	1087.461	2073.082	1318.822	1433.094	486.942	1786.387	-49.110
2000	1095.378	2129.067	1357.945	1542.244	488.845	1854.743	-48.440
2100	1102.364	2182.683	1395.951	1652.138	490.563	1922.991	-47.831
2200	1108.556	2234.111	1432.888	1762.690	492.099	1991.164	-47.275
2300	1114.065	2283.512	1468.805	1873.827	493.451	2059.273	-46.767
2400	1118.984	2331.032	1503.747	1985.484	494.540	2127.270	-46.298
2500	1123.394	2376.802	1537.760	2097.607	495.383	2195.357	-45.869
2600	1127.359	2420.941	1570.884	2210.148	495.940	2263.282	-45.469
2700	1130.936	2463.556	1603.162	2323.065	496.218	2331.278	-45.100
2800	1134.173	2504.745	1634.630	2436.324	496.188	2399.289	-44.758
2900	1137.111	2544.597	1665.325	2549.890	495.819	2467.247	-44.439
3000	1139.784	2583.193	1695.280	2663.737	495.162	2535.256	-44.142
3100	1142.223	2620.606	1724.529	2777.839	494.128	2603.200	-43.863
3200	1144.455	2656.906	1753.102	2892.175	492.767	2671.269	-43.603
3300	1146.500	2692.155	1781.026	3006.724	491.061	2739.434	-43.361
3400	1148.380	2726.409	1808.330	3121.469	488.974	2807.551	-43.132
3500	1150.112	2759.723	1835.039	3236.395	486.516	2875.716	-42.917
3600	1151.709	2792.146	1861.177	3351.487	483.712	2944.060	-42.716
3700	1153.186	2823.722	1886.767	3466.733	480.525	3012.503	-42.528
3800	1154.555	2854.494	1911.830	3582.121	476.929	3080.972	-42.350
3900	1155.825	2884.500	1936.388	3697.640	472.969	3149.475	-42.182
4000	1157.005	2913.778	1960.458	3813.283	468.627	3218.250	-42.025
4100	1158.105	2942.362	1984.059	3929.039	463.863	3287.051	-41.877
4200	1159.130	2970.282	2007.210	4044.901	458.710	3355.964	-41.737
4300	1160.087	2997.568	2029.925	4160.862	453.151	3424.899	-41.603
4400	1160.983	3024.248	2052.222	4276.917	447.197	3494.074	-41.479
4500	1161.822	3050.348	2074.113	4393.057	440.866	3563.451	-41.363
4600	1162.609	3075.892	2095.614	4509.279	434.096	3632.989	-41.253
4700	1163.348	3100.904	2116.738	4625.577	426.906	3702.544	-41.148
4800	1164.043	3125.404	2137.498	4741.947	419.348	3772.381	-41.051
4900	1164.697	3149.412	2157.905	4858.385	411.337	3842.219	-40.958
5000	1165.314	3172.948	2177.971	4974.886	402.982	3912.440	-40.872

3.563. Dinaphtho[2,1,8,7-*defg*:2',1',8',7'-*opqr*]pentacene



Other names: Dinaphtho[2,1,8-*cde*,2',1',8'-*lmn*]perylene
2,3,3',2'-Dipyrenylene

Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 188-91-0
Point Group: C_{2h}

Length: 16.59 Å
Width: 10.32 Å
Breadth: 3.886 Å
L/B Ratio: 1.607

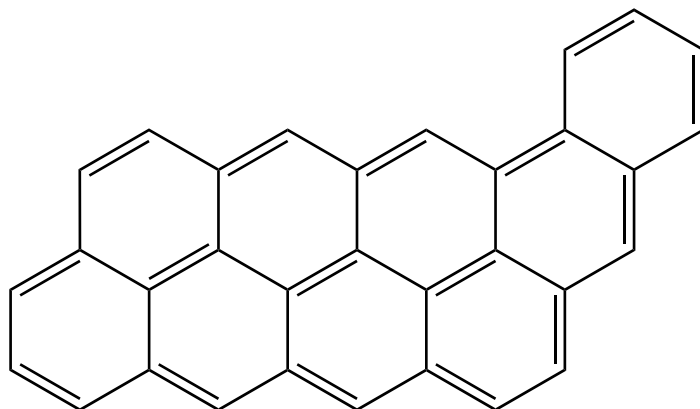
Cartesian coordinates:

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C	-3.4345	1.5387	0.0000	C	2.0390	3.1462	0.0000	H	-4.2093	3.5578	0.0000
C	-4.4599	2.4910	0.0000	C	0.7124	2.7502	0.0000	H	-6.5838	2.8403	0.0000
C	-5.7889	2.0869	0.0000	C	3.0596	2.1893	0.0000	H	-7.1744	0.4313	0.0000
C	-6.1221	0.7372	0.0000	C	5.4301	1.6425	0.0000	H	-2.2937	-4.2120	0.0000
C	-2.0389	-3.1461	0.0000	C	4.4479	2.5726	0.0000	H	0.0881	-3.5064	0.0000
C	-0.7124	-2.7501	0.0000	C	5.1186	0.2360	0.0000	H	-6.4862	-1.9355	0.0000
C	-3.0596	-2.1893	0.0000	C	4.4598	-2.4911	0.0000	H	-4.6844	-3.6429	0.0000
C	-2.7211	-0.8177	0.0000	C	5.7888	-2.0870	0.0000	H	2.2938	4.2121	0.0000
C	-3.7632	0.1648	0.0000	C	6.1221	-0.7372	0.0000	H	-0.0880	3.5065	0.0000
C	-5.1186	-0.2361	0.0000	C	3.4344	-1.5387	0.0000	H	6.4863	1.9354	0.0000
C	-5.4300	-1.6425	0.0000	C	3.7632	-0.1648	0.0000	H	4.6844	3.6429	0.0000
C	-4.4478	-2.5726	0.0000	C	2.7211	0.8177	0.0000	H	4.2091	-3.5578	0.0000
C	-1.3643	-0.4164	0.0000	C	1.3643	0.4165	0.0000	H	6.5838	-2.8403	0.0000
C	-0.3561	-1.3952	0.0000	C	1.0503	-0.9958	0.0000	H	7.1744	-0.4314	0.0000
C	-1.0503	0.9959	0.0000	C	2.0518	-1.9221	0.0000	H	1.8064	-2.9966	0.0000

Table 3.563: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1,8,7-*defg*:2',1',8',7'-*opqr*]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.215	483.037	483.037	∞
100	115.355	355.233	838.176	-48.294	510.199	558.304	-291.622
200	241.929	471.953	625.611	-30.732	495.777	612.171	-159.879
250	314.399	533.678	601.012	-16.833	489.036	642.048	-134.146
298.15	384.585	595.074	595.074	0.000	483.037	672.078	-117.743
300	387.244	597.462	595.082	0.714	482.815	673.249	-117.221
350	457.146	662.459	600.055	21.841	477.278	705.438	-105.279
400	521.991	727.799	611.940	46.344	472.461	738.359	-96.418
450	580.798	792.737	628.428	73.939	468.272	771.853	-89.592
500	633.413	856.707	648.067	104.320	464.621	805.808	-84.180
600	721.663	980.313	693.230	172.250	458.623	874.638	-76.142
700	791.322	1096.996	742.663	248.033	454.166	944.354	-70.467
800	846.969	1206.429	793.869	330.048	451.085	1014.595	-66.245
900	892.093	1308.883	845.463	417.077	449.203	1085.140	-62.979
1000	929.181	1404.855	896.656	508.200	448.357	1155.854	-60.374
1100	960.002	1494.905	946.992	602.705	448.342	1226.622	-58.246
1200	985.850	1579.577	996.215	700.035	449.016	1297.338	-56.470
1300	1007.697	1659.374	1044.187	799.742	450.187	1367.990	-54.965
1400	1026.289	1734.750	1090.846	901.466	451.719	1438.542	-53.672
1500	1042.210	1806.114	1136.173	1004.911	453.532	1508.977	-52.546
1600	1055.922	1873.825	1180.179	1109.834	455.487	1579.274	-51.557
1700	1067.795	1938.205	1222.891	1216.034	457.511	1649.421	-50.679
1800	1078.130	1999.537	1264.347	1323.342	459.523	1719.521	-49.898
1900	1087.169	2058.076	1304.594	1431.617	461.494	1789.449	-49.194
2000	1095.111	2114.047	1343.678	1540.739	463.368	1859.306	-48.559
2100	1102.121	2167.651	1381.647	1650.608	465.061	1929.057	-47.982
2200	1108.332	2219.068	1418.551	1761.137	466.574	1998.734	-47.455
2300	1113.859	2268.459	1454.437	1872.252	467.905	2068.347	-46.973
2400	1118.794	2315.971	1489.351	1983.889	468.974	2137.850	-46.528
2500	1123.217	2361.734	1523.336	2095.993	469.799	2207.444	-46.121
2600	1127.195	2405.866	1556.436	2208.517	470.339	2276.876	-45.742
2700	1130.783	2448.475	1588.690	2321.419	470.601	2346.379	-45.393
2800	1134.030	2489.659	1620.136	2434.663	470.556	2415.899	-45.068
2900	1136.977	2529.506	1650.811	2548.216	470.173	2485.367	-44.765
3000	1139.659	2568.097	1680.747	2662.049	469.503	2554.884	-44.484
3100	1142.106	2605.506	1709.978	2776.140	468.457	2624.338	-44.219
3200	1144.344	2641.803	1738.533	2890.464	467.085	2693.918	-43.973
3300	1146.396	2677.048	1766.441	3005.002	465.367	2763.593	-43.743
3400	1148.282	2711.300	1793.730	3119.737	463.271	2833.221	-43.526
3500	1150.019	2744.611	1820.424	3234.654	460.803	2902.897	-43.322
3600	1151.621	2777.031	1846.548	3349.737	457.990	2972.753	-43.133
3700	1153.103	2808.604	1872.125	3464.974	454.795	3042.707	-42.954
3800	1154.475	2839.374	1897.176	3580.354	451.191	3112.688	-42.786
3900	1155.749	2869.379	1921.721	3695.866	447.223	3182.703	-42.627
4000	1156.934	2898.655	1945.780	3811.500	442.874	3252.990	-42.479
4100	1158.036	2927.236	1969.371	3927.250	438.103	3323.304	-42.339
4200	1159.065	2955.155	1992.511	4043.105	432.942	3393.729	-42.206
4300	1160.025	2982.439	2015.216	4159.060	427.377	3464.177	-42.081
4400	1160.924	3009.118	2037.503	4275.108	421.417	3534.865	-41.963
4500	1161.765	3035.217	2059.385	4391.243	415.080	3605.755	-41.854
4600	1162.554	3060.760	2080.878	4507.459	408.305	3676.806	-41.751
4700	1163.296	3085.770	2101.993	4623.752	401.110	3747.875	-41.652
4800	1163.993	3110.269	2122.745	4740.117	393.546	3819.224	-41.561
4900	1164.649	3134.277	2143.144	4856.550	385.531	3890.576	-41.473
5000	1165.268	3157.812	2163.203	4973.046	377.171	3962.311	-41.393

3.564. Anthra[7,8,9,1,2,3-*rstuvw*x]hexaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-14-8
Point Group: C_s

Length: 17.72 Å
Width: 10.79 Å
Breadth: 3.890 Å
L/B Ratio: 1.642

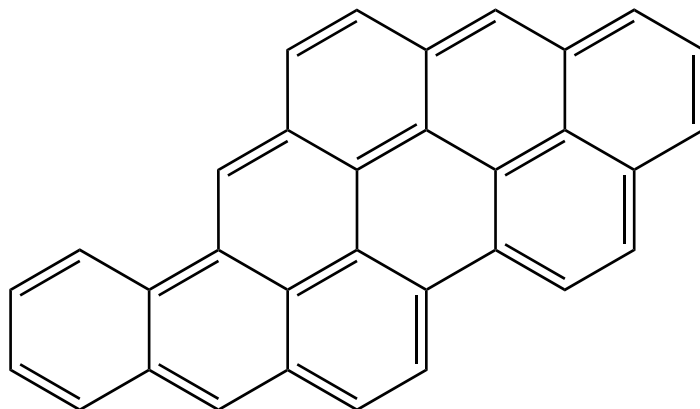
Cartesian coordinates:

C	6.1992	-0.9975	0.0000	C	0.1493	0.0678	0.0000	H	6.9632	-1.7831	0.0000
C	6.5944	0.3529	0.0000	C	-0.2552	-1.2939	0.0000	H	7.6630	0.5929	0.0000
C	5.6614	1.3610	0.0000	C	0.7435	-2.3188	0.0000	H	5.9746	2.4112	0.0000
C	4.2770	1.0569	0.0000	C	1.5376	0.3951	0.0000	H	3.6187	3.1266	0.0000
C	3.2947	2.0786	0.0000	C	2.4945	-0.6262	0.0000	H	1.2619	3.8369	0.0000
C	1.9495	1.7658	0.0000	C	2.0761	-2.0035	0.0000	H	-1.0833	4.5461	0.0000
C	0.9363	2.7892	0.0000	C	3.1035	-3.0268	0.0000	H	-3.4897	3.9730	0.0000
C	-0.3890	2.4731	0.0000	C	4.4130	-2.7102	0.0000	H	-5.2677	2.2909	0.0000
C	-1.4150	3.5011	0.0000	C	4.8580	-1.3312	0.0000	H	-1.9464	-2.6538	0.0000
C	-2.7229	3.1894	0.0000	C	3.8759	-0.2988	0.0000	H	0.4177	-3.3662	0.0000
C	-3.1785	1.8101	0.0000	C	-4.0001	-0.9087	0.0000	H	2.7760	-4.0730	0.0000
C	-4.5071	1.5001	0.0000	C	-4.9434	0.1350	0.0000	H	5.1829	-3.4906	0.0000
C	-2.1862	0.7630	0.0000	C	-6.3219	-0.1727	0.0000	H	-7.0517	0.6449	0.0000
C	-2.5866	-0.5939	0.0000	C	-6.7426	-1.4832	0.0000	H	-7.8114	-1.7208	0.0000
C	-1.6168	-1.6022	0.0000	C	-5.8024	-2.5265	0.0000	H	-6.1486	-3.5652	0.0000
C	-0.8186	1.0908	0.0000	C	-4.4552	-2.2440	0.0000	H	-3.7071	-3.0516	0.0000

Table 3.564: Table of thermodynamic data as a function of temperature for Anthra[7,8,9,1,2,3-*rstuvwx*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-55.639	504.204	504.204	∞
100	116.122	359.177	846.338	-48.716	530.944	578.654	-302.252
200	244.186	476.907	631.902	-30.999	516.677	632.080	-165.079
250	317.163	539.195	607.092	-16.974	510.062	661.695	-138.251
298.15	387.639	601.106	601.106	0.000	504.204	691.447	-121.136
300	390.306	603.512	601.113	0.720	503.988	692.606	-120.591
350	460.316	668.991	606.124	22.003	498.607	724.481	-108.121
400	525.130	734.754	618.094	46.664	493.948	757.064	-98.860
450	583.819	800.056	634.692	74.414	489.914	790.201	-91.722
500	636.270	864.336	654.452	104.942	486.410	823.782	-86.058
600	724.156	988.430	699.866	173.139	480.679	891.824	-77.639
700	793.476	1105.472	749.537	249.154	476.455	960.709	-71.688
800	848.837	1215.173	800.961	331.370	473.574	1030.088	-67.256
900	893.726	1317.833	852.751	418.574	471.866	1099.749	-63.826
1000	930.618	1413.967	904.117	509.850	471.174	1169.559	-61.090
1100	961.275	1504.146	954.609	604.490	471.294	1239.409	-58.853
1200	986.986	1588.922	1003.972	701.940	472.088	1309.196	-56.987
1300	1008.715	1668.805	1052.071	801.755	473.367	1378.909	-55.404
1400	1027.206	1744.254	1098.843	903.575	474.995	1448.514	-54.044
1500	1043.039	1815.677	1144.272	1007.108	476.896	1517.996	-52.860
1600	1056.674	1883.440	1188.371	1112.110	478.930	1587.334	-51.820
1700	1068.481	1947.863	1231.168	1218.382	481.026	1656.517	-50.898
1800	1078.757	2009.233	1272.702	1325.755	483.103	1725.649	-50.076
1900	1087.744	2067.804	1313.020	1434.090	485.134	1794.606	-49.336
2000	1095.640	2123.803	1352.170	1543.268	487.064	1863.489	-48.668
2100	1102.608	2177.432	1390.200	1653.187	488.807	1932.263	-48.061
2200	1108.783	2228.871	1427.160	1763.763	490.367	2000.960	-47.508
2300	1114.276	2278.282	1463.099	1874.921	491.741	2069.593	-47.001
2400	1119.182	2325.810	1498.061	1986.598	492.851	2138.112	-46.534
2500	1123.579	2371.588	1532.092	2098.740	493.713	2206.722	-46.106
2600	1127.532	2415.734	1565.234	2211.299	494.288	2275.167	-45.708
2700	1131.099	2458.356	1597.528	2324.234	494.582	2343.683	-45.340
2800	1134.326	2499.550	1629.012	2437.508	494.568	2412.214	-44.999
2900	1137.255	2539.407	1659.721	2551.089	494.213	2480.692	-44.681
3000	1139.920	2578.008	1689.691	2664.950	493.570	2549.219	-44.385
3100	1142.352	2615.426	1718.953	2779.066	492.550	2617.681	-44.107
3200	1144.576	2651.730	1747.538	2893.414	491.202	2686.269	-43.848
3300	1146.616	2686.982	1775.474	3007.975	489.507	2754.951	-43.606
3400	1148.489	2721.240	1802.789	3122.731	487.431	2823.586	-43.378
3500	1150.215	2754.557	1829.509	3237.668	484.984	2892.267	-43.164
3600	1151.808	2786.982	1855.657	3352.770	482.190	2961.128	-42.964
3700	1153.280	2818.561	1881.257	3468.025	479.013	3030.086	-42.776
3800	1154.644	2849.335	1906.329	3583.422	475.426	3099.071	-42.599
3900	1155.910	2879.344	1930.895	3698.951	471.475	3168.090	-42.431
4000	1157.086	2908.624	1954.974	3814.601	467.141	3237.380	-42.275
4100	1158.182	2937.209	1978.584	3930.365	462.385	3306.698	-42.127
4200	1159.204	2965.131	2001.742	4046.235	457.239	3376.125	-41.987
4300	1160.158	2992.419	2024.465	4162.204	451.688	3445.576	-41.855
4400	1161.051	3019.101	2046.768	4278.265	445.741	3515.265	-41.731
4500	1161.887	3045.202	2068.666	4394.412	439.416	3585.157	-41.615
4600	1162.672	3070.748	2090.174	4510.641	432.653	3655.210	-41.505
4700	1163.408	3095.761	2111.304	4626.945	425.469	3725.279	-41.401
4800	1164.101	3120.262	2132.070	4743.321	417.917	3795.630	-41.304
4900	1164.753	3144.272	2152.483	4859.764	409.912	3865.982	-41.211
5000	1165.368	3167.809	2172.555	4976.270	401.562	3936.717	-41.126

3.565. Benzo[def]pyranthrene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 72986-34-6
Point Group: C_s

Length: 17.99 Å
Width: 10.44 Å
Breadth: 3.885 Å
L/B Ratio: 1.723

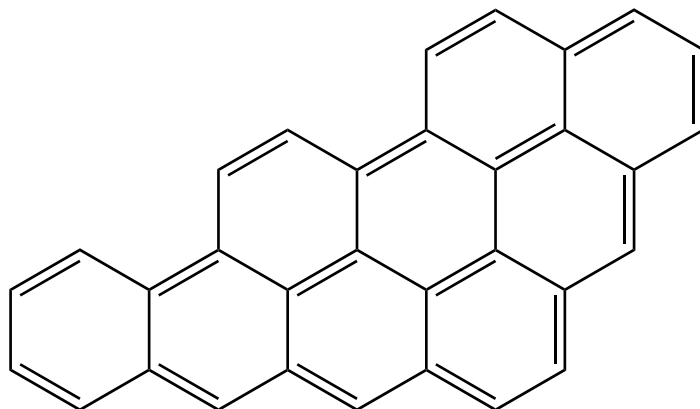
Cartesian coordinates:

C	6.3524	-1.4754	0.0000	C	-2.5631	2.6829	0.0000	H	6.9986	-2.3593	0.0000
C	6.9390	-0.1917	0.0000	C	-3.9089	2.5673	0.0000	H	8.0302	-0.1023	0.0000
C	6.1488	0.9277	0.0000	C	-4.5454	1.2728	0.0000	H	6.5967	1.9280	0.0000
C	4.9889	-1.6120	0.0000	C	-5.9312	1.1387	0.0000	H	4.5175	-2.6068	0.0000
C	4.1458	-0.4716	0.0000	C	-6.5146	-0.1295	0.0000	H	4.3928	2.9573	0.0000
C	4.7338	0.8096	0.0000	C	-5.7307	-1.2692	0.0000	H	2.1828	4.0145	0.0000
C	3.9138	1.9702	0.0000	C	-3.7300	0.1136	0.0000	H	-0.2928	3.8163	0.0000
C	2.5441	1.8605	0.0000	C	-4.3283	-1.1670	0.0000	H	2.7285	-2.7624	0.0000
C	1.6959	3.0323	0.0000	C	-3.4981	-2.3311	0.0000	H	-2.0757	3.6702	0.0000
C	0.3524	2.9240	0.0000	C	-2.3058	0.2378	0.0000	H	-4.5516	3.4551	0.0000
C	-0.3064	1.6377	0.0000	C	-1.5107	-0.9224	0.0000	H	-6.5661	2.0319	0.0000
C	0.5002	0.4667	0.0000	C	-2.1338	-2.2199	0.0000	H	-7.6061	-0.2190	0.0000
C	2.0851	-1.8677	0.0000	C	-1.2762	-3.3898	0.0000	H	-6.1976	-2.2607	0.0000
C	2.7152	-0.5917	0.0000	C	0.0656	-3.2789	0.0000	H	-3.9788	-3.3172	0.0000
C	1.9255	0.5680	0.0000	C	0.7181	-1.9840	0.0000	H	-1.7613	-4.3729	0.0000
C	-1.7013	1.5252	0.0000	C	-0.1024	-0.8081	0.0000	H	0.7060	-4.1686	0.0000

Table 3.565: Table of thermodynamic data as a function of temperature for Benzo[def]pyranthrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-55.588	496.809	496.809	∞
100	116.647	361.358	847.198	-48.584	523.681	571.173	-298.344
200	243.472	479.111	633.465	-30.871	509.410	624.372	-163.066
250	315.817	541.168	608.762	-16.898	502.742	653.882	-136.618
298.15	385.863	602.802	602.802	0.000	496.809	683.545	-119.752
300	388.517	605.197	602.810	0.716	496.589	684.702	-119.215
350	458.276	670.380	607.798	21.904	491.112	716.500	-106.930
400	522.988	735.863	619.715	46.459	486.348	749.020	-97.810
450	581.674	800.911	636.241	74.102	482.206	782.108	-90.783
500	634.182	864.967	655.921	104.523	478.596	815.652	-85.209
600	722.258	988.697	701.163	172.521	472.665	883.650	-76.927
700	791.787	1105.462	750.666	248.357	468.262	952.523	-71.077
800	847.338	1214.951	801.934	330.414	465.222	1021.914	-66.723
900	892.390	1317.443	853.581	417.476	463.372	1091.606	-63.354
1000	929.422	1413.444	904.819	508.625	462.554	1161.461	-60.667
1100	960.201	1503.515	955.195	603.152	462.561	1231.370	-58.472
1200	986.017	1588.202	1004.452	700.500	463.253	1301.224	-56.640
1300	1007.838	1668.012	1052.455	800.223	464.439	1371.013	-55.087
1400	1026.410	1743.398	1099.141	901.960	465.984	1440.701	-53.752
1500	1042.314	1814.769	1144.492	1005.416	467.809	1510.271	-52.591
1600	1056.012	1882.487	1188.519	1110.349	469.774	1579.702	-51.571
1700	1067.875	1946.872	1231.250	1216.557	471.806	1648.982	-50.666
1800	1078.200	2008.209	1272.724	1323.873	473.825	1718.215	-49.860
1900	1087.232	2066.751	1312.986	1432.154	475.803	1787.276	-49.135
2000	1095.167	2122.725	1352.084	1541.283	477.683	1856.265	-48.480
2100	1102.171	2176.331	1390.066	1651.157	479.381	1925.149	-47.884
2200	1108.378	2227.750	1426.982	1761.690	480.899	1993.957	-47.342
2300	1113.900	2277.144	1462.879	1872.809	482.234	2062.702	-46.844
2400	1118.832	2324.657	1497.803	1984.451	483.307	2131.336	-46.386
2500	1123.252	2370.421	1531.798	2096.559	484.135	2200.062	-45.967
2600	1127.227	2414.555	1564.906	2209.086	484.679	2268.625	-45.576
2700	1130.813	2457.165	1597.168	2321.991	484.944	2337.259	-45.216
2800	1134.058	2498.350	1628.622	2435.237	484.902	2405.910	-44.882
2900	1137.003	2538.198	1659.304	2548.793	484.521	2474.508	-44.570
3000	1139.683	2576.790	1689.247	2662.629	483.854	2543.157	-44.279
3100	1142.128	2614.200	1718.483	2776.721	482.810	2611.741	-44.007
3200	1144.365	2650.497	1747.045	2891.048	481.440	2680.452	-43.753
3300	1146.415	2685.743	1774.959	3005.588	479.725	2749.257	-43.516
3400	1148.300	2719.995	1802.252	3120.325	477.630	2818.016	-43.293
3500	1150.036	2753.307	1828.952	3235.243	475.164	2886.822	-43.083
3600	1151.637	2785.727	1855.080	3350.328	472.352	2955.808	-42.887
3700	1153.118	2817.301	1880.662	3465.567	469.159	3024.893	-42.703
3800	1154.490	2848.071	1905.717	3580.948	465.556	3094.004	-42.529
3900	1155.763	2878.076	1930.266	3696.461	461.590	3163.149	-42.365
4000	1156.946	2907.353	1954.329	3812.097	457.242	3232.566	-42.212
4100	1158.048	2935.935	1977.923	3927.848	452.472	3302.011	-42.067
4200	1159.076	2963.853	2001.066	4043.705	447.313	3371.566	-41.931
4300	1160.036	2991.138	2023.775	4159.661	441.749	3441.144	-41.801
4400	1160.934	3017.817	2046.065	4275.710	435.790	3510.962	-41.680
4500	1161.775	3043.916	2067.951	4391.846	429.454	3580.983	-41.566
4600	1162.564	3069.460	2089.446	4508.063	422.680	3651.164	-41.459
4700	1163.305	3094.470	2110.564	4624.357	415.485	3721.362	-41.357
4800	1164.002	3118.969	2131.318	4740.723	407.923	3791.842	-41.263
4900	1164.658	3142.977	2151.720	4857.156	399.908	3862.324	-41.172
5000	1165.276	3166.512	2171.782	4973.653	391.549	3933.189	-41.089

3.566. Phenanthro[2,1,10,9,8,7-*tuvwxyz*]hexaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120836-17-1
Point Group: C_s

Length: 18.01 Å
Width: 10.45 Å
Breadth: 3.887 Å
L/B Ratio: 1.724

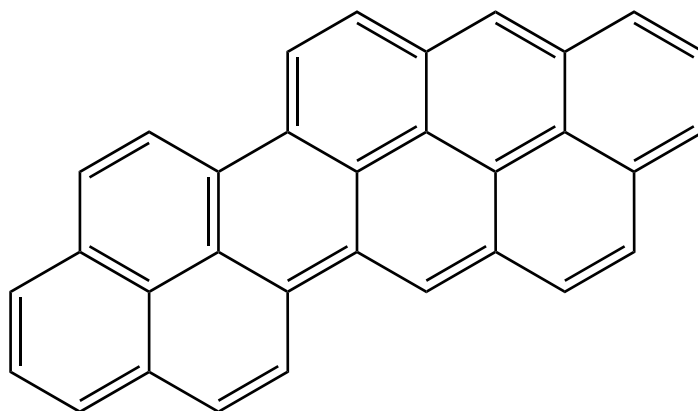
Cartesian coordinates:

C	6.4704	-1.6608	0.0000	C	0.5365	0.0049	0.0000	H	7.1573	-2.5134	0.0000
C	6.9987	-0.3497	0.0000	C	-0.0157	-1.2947	0.0000	H	8.0850	-0.2124	0.0000
C	6.1604	0.7319	0.0000	C	0.8735	-2.4171	0.0000	H	6.5622	1.7516	0.0000
C	5.1163	-1.8596	0.0000	C	2.2203	-2.2478	0.0000	H	4.6884	-2.8738	0.0000
C	4.2208	-0.7572	0.0000	C	2.8022	-0.9400	0.0000	H	4.3115	2.6781	0.0000
C	4.7498	0.5509	0.0000	C	1.9581	0.1773	0.0000	H	2.0648	3.6347	0.0000
C	3.8797	1.6694	0.0000	C	-4.5207	0.6589	0.0000	H	-0.1825	4.6058	0.0000
C	2.5118	1.4979	0.0000	C	-5.9083	0.4872	0.0000	H	-2.6388	4.3130	0.0000
C	1.6213	2.6311	0.0000	C	-6.4578	-0.7904	0.0000	H	-4.5974	2.8387	0.0000
C	0.2709	2.4674	0.0000	C	-5.6425	-1.9141	0.0000	H	0.4252	-3.4227	0.0000
C	-0.6318	3.6058	0.0000	C	-3.6804	-0.4806	0.0000	H	2.9046	-3.1102	0.0000
C	-1.9669	3.4468	0.0000	C	-4.2496	-1.7740	0.0000	H	-6.5636	1.3656	0.0000
C	-2.5756	2.1279	0.0000	C	-3.3766	-2.9162	0.0000	H	-7.5464	-0.9105	0.0000
C	-3.9296	1.9683	0.0000	C	-2.0309	-2.7628	0.0000	H	-6.0858	-2.9163	0.0000
C	-1.6986	0.9783	0.0000	C	-1.4232	-1.4602	0.0000	H	-3.8302	-3.9139	0.0000
C	-0.3106	1.1410	0.0000	C	-2.2571	-0.3248	0.0000	H	-1.3571	-3.6336	0.0000

Table 3.566: Table of thermodynamic data as a function of temperature for Phenanthro[2,1,10,9,8,7-tuvwxyz]hexaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-55.824	499.983	499.983	∞
100	117.388	363.476	850.940	-48.746	526.693	573.973	-299.807
200	244.300	481.752	636.538	-30.957	512.498	626.931	-163.734
250	316.704	544.001	611.768	-16.942	505.873	656.305	-137.125
298.15	386.768	605.794	605.794	0.000	499.983	685.828	-120.152
300	389.422	608.194	605.801	0.718	499.765	686.979	-119.611
350	459.166	673.516	610.801	21.950	494.333	718.623	-107.246
400	523.843	739.115	622.741	46.550	489.612	750.984	-98.066
450	582.482	804.261	639.298	74.234	485.513	783.907	-90.992
500	634.938	868.400	659.011	104.694	481.941	817.281	-85.379
600	722.908	992.259	704.322	172.762	476.081	884.929	-77.038
700	792.342	1109.116	753.890	248.659	471.738	953.441	-71.145
800	847.812	1218.673	805.215	330.766	468.749	1022.463	-66.759
900	892.799	1321.218	856.915	417.873	466.944	1091.780	-63.364
1000	929.777	1417.259	908.199	509.060	466.163	1161.256	-60.657
1100	960.510	1507.361	958.616	603.620	466.203	1230.781	-58.444
1200	986.289	1592.074	1007.910	700.997	466.924	1300.250	-56.597
1300	1008.079	1671.904	1055.946	800.745	468.136	1369.650	-55.032
1400	1026.624	1747.307	1102.661	902.505	469.704	1438.948	-53.687
1500	1042.505	1818.692	1148.038	1005.982	471.548	1508.126	-52.517
1600	1056.184	1886.421	1192.089	1110.933	473.532	1577.165	-51.488
1700	1068.030	1950.816	1234.841	1217.157	475.580	1646.050	-50.576
1800	1078.341	2012.162	1276.335	1324.488	477.615	1714.888	-49.764
1900	1087.360	2070.711	1316.615	1432.783	479.606	1783.554	-49.032
2000	1095.285	2126.692	1355.730	1541.923	481.498	1852.147	-48.372
2100	1102.279	2180.303	1393.728	1651.809	483.207	1920.634	-47.772
2200	1108.477	2231.727	1430.658	1762.352	484.735	1989.044	-47.225
2300	1113.992	2281.125	1466.568	1873.481	486.080	2057.392	-46.724
2400	1118.917	2328.642	1501.504	1985.131	487.162	2125.627	-46.262
2500	1123.331	2374.410	1535.511	2097.247	487.998	2193.954	-45.839
2600	1127.300	2418.546	1568.630	2209.782	488.549	2262.118	-45.446
2700	1130.881	2461.159	1600.902	2322.695	488.821	2330.353	-45.082
2800	1134.122	2502.346	1632.365	2435.947	488.786	2398.604	-44.746
2900	1137.062	2542.196	1663.055	2549.509	488.412	2466.803	-44.431
3000	1139.739	2580.790	1693.006	2663.351	487.750	2535.052	-44.138
3100	1142.181	2618.202	1722.251	2777.449	486.712	2603.236	-43.863
3200	1144.414	2654.501	1750.820	2891.780	485.347	2671.546	-43.608
3300	1146.462	2689.748	1778.740	3006.326	483.636	2739.951	-43.369
3400	1148.344	2724.002	1806.041	3121.067	481.546	2808.309	-43.144
3500	1150.078	2757.315	1832.746	3235.989	479.084	2876.714	-42.932
3600	1151.677	2789.736	1858.881	3351.078	476.277	2945.300	-42.734
3700	1153.156	2821.311	1884.468	3466.321	473.088	3013.983	-42.549
3800	1154.526	2852.083	1909.528	3581.706	469.489	3082.693	-42.374
3900	1155.797	2882.089	1934.083	3697.223	465.526	3151.438	-42.208
4000	1156.979	2911.366	1958.150	3812.862	461.181	3220.454	-42.054
4100	1158.079	2939.948	1981.749	3928.616	456.415	3289.497	-41.908
4200	1159.106	2967.868	2004.897	4044.476	451.258	3358.651	-41.770
4300	1160.064	2995.153	2027.610	4160.435	445.698	3427.827	-41.639
4400	1160.961	3021.833	2049.904	4276.486	439.741	3497.244	-41.517
4500	1161.801	3047.933	2071.794	4392.625	433.408	3566.863	-41.402
4600	1162.589	3073.477	2093.293	4508.845	426.636	3636.642	-41.295
4700	1163.329	3098.487	2114.415	4625.141	419.444	3706.439	-41.192
4800	1164.025	3122.987	2135.172	4741.509	411.884	3776.517	-41.096
4900	1164.680	3146.995	2155.578	4857.945	403.872	3846.597	-41.004
5000	1165.297	3170.531	2175.642	4974.444	395.515	3917.060	-40.920

3.567. Dinaphtho[8,1,2-*cde*:7',8',1',2',3'-*pqrst*]pentaphene



Formula: C₃₂H₁₆
Mass: 400.469 g/mol
CAS Number: 120835-97-4
Point Group: C_s

Length: 17.93 Å
Width: 10.36 Å
Breadth: 3.885 Å
L/B Ratio: 1.731

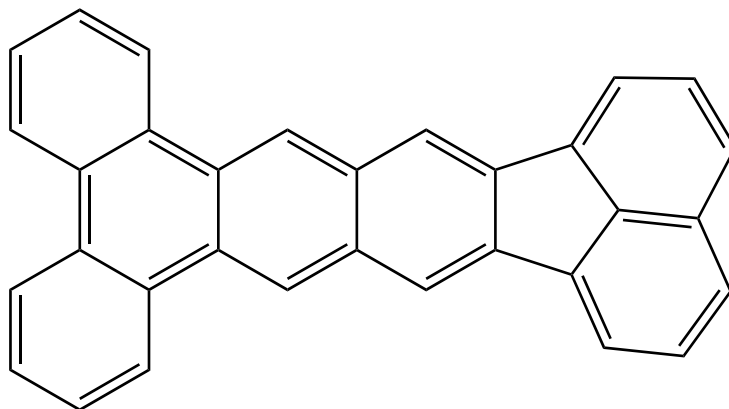
Cartesian coordinates:

C	4.3186	-2.2597	0.0000	C	-1.6277	-0.6667	0.0000	H	5.0169	-3.1045	0.0000
C	2.9836	-2.4599	0.0000	C	-2.1624	-1.9982	0.0000	H	2.5626	-3.4772	0.0000
C	2.0487	-1.3599	0.0000	C	-1.2323	-3.1058	0.0000	H	-0.2069	2.9812	0.0000
C	0.2874	0.8673	0.0000	C	0.0994	-2.8983	0.0000	H	-2.5020	3.8808	0.0000
C	-0.6218	1.9604	0.0000	C	0.6672	-1.5682	0.0000	H	-4.9506	3.5006	0.0000
C	-1.9812	1.7598	0.0000	C	-0.2168	-0.4537	0.0000	H	-6.8651	1.9470	0.0000
C	-2.9157	2.8657	0.0000	C	4.8685	-0.9264	0.0000	H	-7.7581	-0.3646	0.0000
C	-4.2483	2.6590	0.0000	C	6.2448	-0.7076	0.0000	H	-6.2229	-2.3141	0.0000
C	-4.8025	1.3221	0.0000	C	6.7498	0.5918	0.0000	H	-3.9304	-3.2202	0.0000
C	-6.1707	1.0992	0.0000	C	5.8946	1.6811	0.0000	H	-1.6456	-4.1211	0.0000
C	-6.6739	-0.2098	0.0000	C	3.9817	0.1776	0.0000	H	0.8051	-3.7435	0.0000
C	-5.8234	-1.2936	0.0000	C	4.5047	1.4889	0.0000	H	6.9318	-1.5614	0.0000
C	-3.9119	0.2141	0.0000	C	3.5957	2.5994	0.0000	H	7.8335	0.7498	0.0000
C	-4.4242	-1.1019	0.0000	C	2.2557	2.3965	0.0000	H	6.2980	2.7000	0.0000
C	-3.5214	-2.2023	0.0000	C	1.6962	1.0746	0.0000	H	4.0128	3.6129	0.0000
C	-2.5030	0.4265	0.0000	C	2.5621	-0.0318	0.0000	H	1.5546	3.2454	0.0000

Table 3.567: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*cde*:7',8',1',2',3'-*pqrst*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-55.906	495.429	495.429	∞
100	117.194	366.231	854.253	-48.802	522.083	569.088	-297.255
200	244.615	484.493	639.553	-31.012	507.889	621.775	-162.388
250	317.282	546.843	614.737	-16.974	501.288	651.009	-136.018
298.15	387.508	608.752	608.752	0.000	495.429	680.392	-119.199
300	390.167	611.157	608.759	0.719	495.213	681.537	-118.664
350	460.005	676.601	613.768	21.992	489.821	713.031	-106.412
400	524.724	742.316	625.731	46.634	485.143	745.234	-97.316
450	583.370	807.567	642.317	74.362	481.088	777.995	-90.305
500	635.809	871.798	662.064	104.867	477.560	811.201	-84.744
600	723.705	995.810	707.445	173.019	471.784	878.501	-76.479
700	793.044	1112.783	757.083	248.990	467.515	946.652	-70.639
800	848.421	1222.428	808.474	331.163	464.592	1015.303	-66.291
900	893.323	1325.039	860.232	418.326	462.843	1084.240	-62.926
1000	930.229	1421.131	911.569	509.562	462.111	1153.332	-60.243
1100	960.902	1511.274	962.033	604.165	462.194	1222.468	-58.049
1200	986.630	1596.019	1011.370	701.578	462.951	1291.543	-56.218
1300	1008.377	1675.874	1059.444	801.358	464.195	1360.548	-54.666
1400	1026.887	1751.298	1106.194	903.146	465.791	1429.448	-53.332
1500	1042.738	1822.700	1151.602	1006.647	467.660	1498.226	-52.172
1600	1056.392	1890.444	1195.681	1111.620	469.666	1566.863	-51.152
1700	1068.216	1954.850	1238.459	1217.865	471.734	1635.346	-50.247
1800	1078.509	2016.206	1279.977	1325.213	473.786	1703.780	-49.441
1900	1087.511	2074.764	1320.278	1433.523	475.793	1772.041	-48.716
2000	1095.422	2130.752	1359.412	1542.679	477.700	1840.228	-48.061
2100	1102.404	2184.370	1397.429	1652.577	479.422	1908.308	-47.466
2200	1108.592	2235.799	1434.375	1763.133	480.962	1976.312	-46.923
2300	1114.097	2285.202	1470.301	1874.273	482.318	2044.252	-46.425
2400	1119.014	2332.723	1505.252	1985.933	483.410	2112.080	-45.967
2500	1123.420	2378.495	1539.271	2098.058	484.256	2179.998	-45.548
2600	1127.383	2422.635	1572.403	2210.602	484.815	2247.754	-45.157
2700	1130.958	2465.251	1604.687	2323.522	485.095	2315.580	-44.797
2800	1134.194	2506.440	1636.161	2436.782	485.067	2383.421	-44.462
2900	1137.130	2546.293	1666.862	2550.351	484.700	2451.211	-44.150
3000	1139.802	2584.889	1696.823	2664.199	484.045	2519.050	-43.860
3100	1142.240	2622.303	1726.076	2778.303	483.013	2586.824	-43.587
3200	1144.470	2658.604	1754.653	2892.640	481.654	2654.724	-43.333
3300	1146.515	2693.853	1782.583	3007.191	479.948	2722.719	-43.096
3400	1148.394	2728.108	1809.891	3121.938	477.863	2790.666	-42.872
3500	1150.124	2761.422	1836.604	3236.865	475.406	2858.660	-42.662
3600	1151.721	2793.845	1862.745	3351.958	472.603	2926.836	-42.466
3700	1153.197	2825.421	1888.339	3467.205	469.418	2995.108	-42.282
3800	1154.565	2856.193	1913.405	3582.594	465.823	3063.407	-42.109
3900	1155.835	2886.200	1937.966	3698.115	461.864	3131.740	-41.944
4000	1157.015	2915.479	1962.039	3813.758	457.523	3200.345	-41.791
4100	1158.113	2944.062	1985.644	3929.515	452.760	3268.976	-41.646
4200	1159.138	2971.982	2008.797	4045.378	447.607	3337.719	-41.510
4300	1160.095	2999.269	2031.515	4161.340	442.050	3406.484	-41.380
4400	1160.991	3025.949	2053.814	4277.395	436.096	3475.489	-41.258
4500	1161.829	3052.049	2075.708	4393.537	429.766	3544.696	-41.145
4600	1162.616	3077.594	2097.211	4509.759	422.997	3614.064	-41.038
4700	1163.355	3102.605	2118.337	4626.058	415.808	3683.449	-40.936
4800	1164.049	3127.105	2139.099	4742.429	408.250	3753.115	-40.841
4900	1164.703	3151.114	2159.508	4858.867	400.240	3822.783	-40.751
5000	1165.320	3174.650	2179.577	4975.368	391.886	3892.835	-40.667

3.568. Fluorantheno[8,9-*b*]triphenylene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 24754-03-8
Point Group: C_{2v}

Length: 17.61 Å
Width: 11.59 Å
Breadth: 3.887 Å
L/B Ratio: 1.518

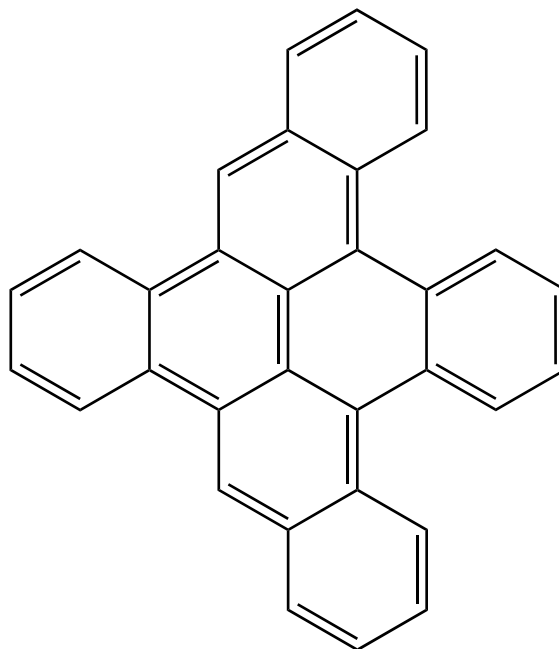
Cartesian coordinates:

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C	3.5261	-2.7975	0.0000	C	-1.4547	-1.4463	0.0000	H	6.8314	0.9678	0.0000
C	4.7310	-3.4746	0.0000	C	-2.6266	-0.7594	0.0000	H	6.8076	3.4542	0.0000
C	3.4864	-1.3929	0.0000	C	-2.6435	0.6985	0.0000	H	4.6400	4.6779	0.0000
C	4.6935	-0.6743	0.0000	C	-4.0170	-1.2305	0.0000	H	2.4988	3.4141	0.0000
C	3.4532	1.4733	0.0000	C	-6.8311	-1.3573	0.0000	H	0.9681	2.5057	0.0000
C	4.6767	0.7828	0.0000	C	-6.0542	-2.4908	0.0000	H	1.0259	-2.4826	0.0000
C	5.8761	1.5145	0.0000	C	-4.6315	-2.4519	0.0000	H	-1.4893	2.5078	0.0000
C	5.8654	2.8967	0.0000	C	-4.8303	-0.0559	0.0000	H	-1.4308	-2.5415	0.0000
C	4.6494	3.5832	0.0000	C	-4.0445	1.1372	0.0000	H	-7.9242	-1.4251	0.0000
C	3.4604	2.8784	0.0000	C	-4.6872	2.3440	0.0000	H	-6.5377	-3.4740	0.0000
C	2.2113	-0.6855	0.0000	C	-6.1104	2.3499	0.0000	H	-4.0584	-3.3842	0.0000
C	2.1949	0.7366	0.0000	C	-6.8608	1.1986	0.0000	H	-4.1360	3.2894	0.0000
C	0.9794	1.4037	0.0000	C	-6.2193	-0.0721	0.0000	H	-6.6166	3.3216	0.0000
C	1.0116	-1.3806	0.0000	H	6.8856	-3.2956	0.0000	H	-7.9551	1.2410	0.0000
C	-0.2249	-0.7100	0.0000	H	6.8520	-0.8094	0.0000				

Table 3.568: Table of thermodynamic data as a function of temperature for Fluorantheno[8,9-*b*]triphenylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	–59.696	554.533	554.533	∞
100	132.201	381.300	897.068	–51.577	583.880	639.450	–334.008
200	257.811	509.254	671.256	–32.400	568.378	701.194	–183.129
250	331.315	574.617	645.361	–17.686	561.056	735.244	–153.618
298.15	403.154	639.128	639.128	0.000	554.533	769.401	–134.793
300	405.883	641.630	639.135	0.748	554.292	770.732	–134.194
350	477.690	709.644	644.343	22.855	548.286	807.295	–120.480
400	544.341	777.847	656.770	48.431	543.084	844.649	–110.298
450	604.757	845.512	673.990	77.185	538.593	882.620	–102.450
500	658.782	912.081	694.482	108.800	534.714	921.082	–96.223
600	749.396	1040.529	741.548	179.389	528.446	998.978	–86.967
700	821.040	1161.640	793.001	258.047	523.927	1077.788	–80.424
800	878.466	1275.159	846.254	343.124	520.955	1157.119	–75.551
900	925.228	1381.418	899.878	433.386	519.330	1236.732	–71.777
1000	963.828	1480.961	953.063	527.898	518.871	1316.478	–68.764
1100	996.038	1574.380	1005.344	625.939	519.353	1396.233	–66.300
1200	1023.151	1662.242	1056.461	726.936	520.616	1475.888	–64.242
1300	1046.141	1745.070	1106.276	830.432	522.455	1555.427	–62.497
1400	1065.759	1823.334	1154.725	936.052	524.719	1634.811	–60.994
1500	1082.599	1897.453	1201.792	1043.491	527.318	1714.024	–59.686
1600	1097.132	1967.797	1247.488	1152.495	530.103	1793.045	–58.536
1700	1109.739	2034.698	1291.843	1262.854	532.991	1871.861	–57.514
1800	1120.728	2098.447	1334.897	1374.389	535.897	1950.580	–56.603
1900	1130.352	2159.305	1376.698	1486.954	538.785	2029.077	–55.782
2000	1138.818	2217.504	1417.294	1600.421	541.595	2107.454	–55.040
2100	1146.297	2273.252	1456.736	1714.685	544.236	2185.678	–54.365
2200	1152.930	2326.734	1495.074	1829.653	546.709	2263.783	–53.748
2300	1158.836	2378.117	1532.357	1945.247	549.008	2341.778	–53.182
2400	1164.114	2427.550	1568.634	2061.399	551.051	2419.622	–52.661
2500	1168.847	2475.169	1603.948	2178.051	552.854	2497.519	–52.182
2600	1173.106	2521.096	1638.345	2295.153	554.373	2575.212	–51.736
2700	1176.949	2565.443	1671.866	2412.659	555.615	2652.937	–51.323
2800	1180.429	2608.310	1704.549	2530.530	556.550	2730.647	–50.940
2900	1183.588	2649.789	1736.432	2648.734	557.143	2808.266	–50.581
3000	1186.464	2689.963	1767.551	2767.239	557.447	2885.902	–50.247
3100	1189.089	2728.911	1797.937	2886.018	557.371	2963.443	–49.933
3200	1191.490	2766.701	1827.624	3005.049	556.963	3041.078	–49.639
3300	1193.693	2803.400	1856.639	3124.310	556.204	3118.777	–49.365
3400	1195.717	2839.065	1885.012	3243.782	555.060	3196.403	–49.106
3500	1197.582	2873.754	1912.768	3363.448	553.537	3274.047	–48.861
3600	1199.303	2907.515	1939.934	3483.293	551.662	3351.843	–48.633
3700	1200.895	2940.397	1966.531	3603.304	549.397	3429.715	–48.418
3800	1202.370	2972.442	1992.582	3723.468	546.712	3507.584	–48.214
3900	1203.738	3003.692	2018.109	3843.774	543.655	3585.467	–48.021
4000	1205.011	3034.184	2043.131	3964.213	540.207	3663.597	–47.841
4100	1206.196	3063.954	2067.668	4084.774	536.327	3741.731	–47.669
4200	1207.302	3093.034	2091.736	4205.449	532.048	3819.955	–47.507
4300	1208.334	3121.455	2115.354	4326.232	527.352	3898.180	–47.353
4400	1209.300	3149.245	2138.537	4447.114	522.251	3976.627	–47.208
4500	1210.205	3176.431	2161.300	4568.090	516.762	4055.259	–47.071
4600	1211.054	3203.040	2183.659	4689.153	510.824	4134.028	–46.942
4700	1211.852	3229.094	2205.626	4810.299	504.453	4212.797	–46.819
4800	1212.601	3254.615	2227.215	4931.522	497.705	4291.831	–46.704
4900	1213.307	3279.625	2248.438	5052.818	490.493	4370.850	–46.593
5000	1213.973	3304.144	2269.308	5174.182	482.927	4450.240	–46.490

3.569. Benzo[*h*]naphtho[1,2,3,4-*rst*]pentaphene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 31541-02-3
Point Group: C₂

Length: 16.01 Å
Width: 14.12 Å
Breadth: 4.780 Å
L/B Ratio: 1.134

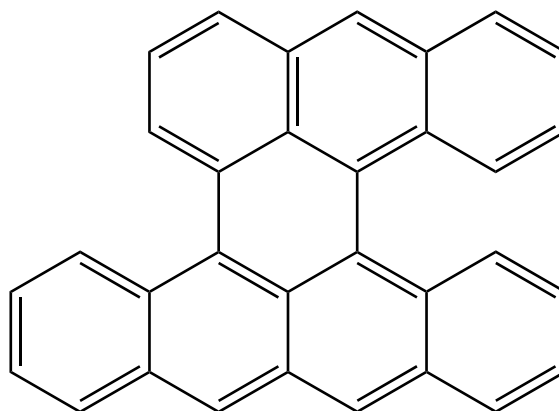
Cartesian coordinates:

C	-2.7856	-1.5712	-0.2829	C	0.6459	4.5659	0.2749	H	-2.4651	-4.0534	-0.3139
C	-1.4214	-1.5597	-0.1391	C	-0.6458	4.5662	-0.2675	H	-1.2351	-6.1997	-0.1598
C	1.4216	-1.5599	0.1385	C	-1.3006	3.3704	-0.4485	H	1.2338	-6.1997	0.1697
C	2.7862	-1.5717	0.2783	C	-3.5410	-0.3790	-0.1734	H	2.4646	-4.0536	0.3185
C	-0.7216	-0.3091	-0.0451	C	-2.8804	0.8517	0.0193	H	2.3226	3.3808	0.8571
C	0.7218	-0.3091	0.0462	C	-3.6957	1.9631	0.3659	H	1.1333	5.5118	0.5314
C	1.4405	0.8922	0.0711	C	-5.0633	1.8753	0.3936	H	-1.1328	5.5125	-0.5236
C	-1.4402	0.8923	-0.0696	C	-5.7105	0.6631	0.0796	H	-2.3220	3.3818	-0.8525
C	0.6951	-2.8255	0.0856	C	-4.9594	-0.4498	-0.1854	H	-3.2245	2.9171	0.6381
C	-0.6954	-2.8255	-0.0837	C	2.8805	0.8517	-0.0205	H	-5.6661	2.7475	0.6680
C	-1.3737	-4.0513	-0.1739	C	3.5415	-0.3795	0.1679	H	-6.8042	0.6191	0.0722
C	-0.6915	-5.2522	-0.0874	C	4.9598	-0.4508	0.1756	H	-5.4395	-1.4126	-0.3951
C	0.6905	-5.2522	0.0951	C	5.7106	0.6626	-0.0885	H	5.4403	-1.4142	0.3816
C	1.3731	-4.0513	0.1786	C	5.0628	1.8759	-0.3970	H	6.8042	0.6182	-0.0840
C	-0.6933	2.1341	-0.1282	C	3.6954	1.9638	-0.3659	H	5.6652	2.7489	-0.6697
C	0.6935	2.1339	0.1322	H	-3.3215	-2.5227	-0.4307	H	3.2239	2.9191	-0.6332
C	1.3006	3.3698	0.4545	H	3.3225	-2.5233	0.4240				

Table 3.569: Table of thermodynamic data as a function of temperature for Benzo[*h*]naphtho[1,2,3,4-*rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-59.244	586.896	586.896	∞
100	129.847	376.013	889.728	-51.371	616.449	672.548	-351.296
200	256.972	503.064	664.648	-32.317	600.825	734.879	-191.927
250	330.450	568.236	638.818	-17.645	593.461	769.244	-160.721
298.15	402.342	632.598	632.598	0.000	586.896	803.711	-140.804
300	405.075	635.095	632.606	0.747	586.654	805.055	-140.170
350	477.034	702.995	637.804	22.817	580.611	841.947	-125.651
400	543.877	771.123	650.213	48.364	575.381	879.636	-114.866
450	604.478	838.745	667.412	77.100	570.872	917.944	-106.550
500	658.654	905.292	687.883	108.705	566.983	956.745	-99.948
600	749.449	1033.736	734.917	179.291	560.712	1035.320	-90.131
700	821.149	1154.860	786.348	257.959	556.202	1114.809	-83.186
800	878.560	1268.393	839.585	343.046	553.240	1194.817	-78.012
900	925.279	1374.661	893.199	433.315	551.623	1275.106	-74.004
1000	963.831	1474.207	946.376	527.831	551.167	1355.527	-70.804
1100	995.998	1567.623	998.651	625.869	551.646	1435.959	-68.187
1200	1023.076	1655.481	1049.763	726.861	552.904	1516.289	-66.001
1300	1046.040	1738.302	1099.573	830.347	554.733	1596.504	-64.147
1400	1065.641	1816.558	1148.017	935.957	556.987	1676.566	-62.552
1500	1082.469	1890.668	1195.079	1043.383	559.573	1756.457	-61.164
1600	1096.995	1961.004	1240.770	1152.374	562.345	1836.157	-59.943
1700	1109.599	2027.896	1285.120	1262.718	565.219	1915.652	-58.860
1800	1120.588	2091.637	1328.170	1374.240	568.111	1995.052	-57.894
1900	1130.214	2152.487	1369.966	1486.791	570.986	2074.231	-57.023
2000	1138.683	2210.680	1410.558	1600.244	573.781	2153.290	-56.237
2100	1146.165	2266.421	1449.995	1714.494	576.409	2232.196	-55.522
2200	1152.803	2319.897	1488.329	1829.449	578.869	2310.985	-54.869
2300	1158.714	2371.274	1525.608	1945.031	581.156	2389.664	-54.270
2400	1163.996	2420.702	1561.881	2061.171	583.187	2468.193	-53.718
2500	1168.734	2468.316	1597.192	2177.812	584.978	2546.774	-53.211
2600	1172.998	2514.240	1631.585	2294.902	586.486	2625.153	-52.739
2700	1176.846	2558.582	1665.102	2412.398	587.718	2703.564	-52.303
2800	1180.330	2601.445	1697.781	2530.259	588.642	2781.960	-51.897
2900	1183.494	2642.921	1729.661	2648.453	589.226	2860.266	-51.518
3000	1186.374	2683.092	1760.776	2766.949	589.521	2938.589	-51.164
3100	1189.003	2722.037	1791.160	2885.719	589.435	3016.817	-50.832
3200	1191.408	2759.825	1820.843	3004.742	589.020	3095.139	-50.522
3300	1193.614	2796.520	1849.856	3123.994	588.252	3173.527	-50.232
3400	1195.642	2832.184	1878.226	3243.459	587.101	3251.840	-49.957
3500	1197.510	2866.870	1905.979	3363.117	585.570	3330.172	-49.699
3600	1199.234	2900.629	1933.142	3482.956	583.688	3408.657	-49.457
3700	1200.829	2933.509	1959.736	3602.960	581.416	3487.218	-49.230
3800	1202.306	2965.553	1985.785	3723.118	578.725	3565.775	-49.014
3900	1203.678	2996.801	2011.310	3843.418	575.662	3644.347	-48.810
4000	1204.953	3027.292	2036.330	3963.850	572.208	3723.167	-48.619
4100	1206.140	3057.060	2060.864	4084.405	568.322	3801.990	-48.437
4200	1207.248	3086.139	2084.931	4205.075	564.037	3880.904	-48.265
4300	1208.283	3114.558	2108.546	4325.852	559.336	3959.818	-48.101
4400	1209.251	3142.347	2131.727	4446.730	554.231	4038.954	-47.947
4500	1210.158	3169.533	2154.488	4567.701	548.737	4118.276	-47.803
4600	1211.008	3196.140	2176.845	4688.759	542.793	4197.736	-47.666
4700	1211.807	3222.193	2198.810	4809.900	536.418	4277.195	-47.535
4800	1212.559	3247.714	2220.397	4931.119	529.666	4356.918	-47.412
4900	1213.266	3272.723	2241.619	5052.411	522.450	4436.627	-47.294
5000	1213.933	3297.241	2262.487	5173.771	514.879	4516.708	-47.185

3.570. Tribenzo[*a,f,j*]perylene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 117440-50-3
Point Group: C₁

Length: 15.27 Å
Width: 12.65 Å
Breadth: 6.939 Å
L/B Ratio: 1.207

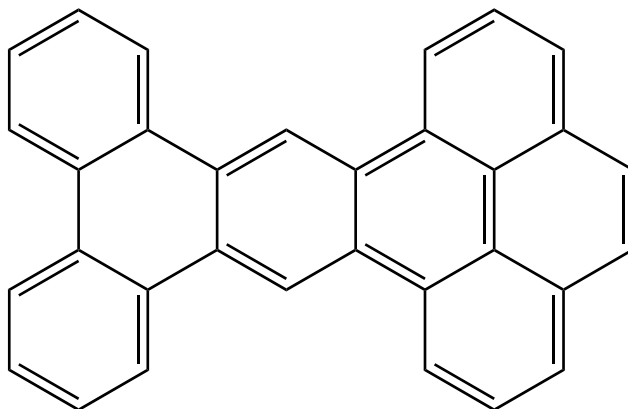
Cartesian coordinates:

C	1.2374	-1.4342	-0.6455	C	5.3309	-0.8589	0.8463	H	3.0666	-2.1986	-1.4772
C	0.1510	-3.9283	-1.4186	C	5.7862	0.4593	1.1461	H	-2.4100	-4.2749	-0.6307
C	1.4409	-3.6116	-1.7148	C	4.9316	1.5070	1.0483	H	3.0889	3.4121	0.7418
C	1.9965	-2.3729	-1.2985	C	-1.3490	1.8171	-0.4553	H	0.8723	4.3288	0.3080
C	-0.1721	-1.6796	-0.4833	C	-0.8221	3.1371	-0.2952	H	3.7238	-2.0990	0.2119
C	-1.0377	-0.6592	-0.0467	C	-1.6692	4.2709	-0.5529	H	6.0320	-1.6930	0.9550
C	-1.9994	-3.2838	-0.4023	C	-2.9335	4.1015	-1.0131	H	6.8257	0.6019	1.4582
C	-0.6872	-2.9738	-0.7602	C	-3.4388	2.7878	-1.2525	H	5.2593	2.5268	1.2814
C	1.7742	-0.1867	-0.0967	C	-2.6821	1.6944	-0.9800	H	-1.2590	5.2722	-0.3791
C	2.7137	2.3985	0.5526	C	-2.7771	-2.3473	0.2852	H	-3.5802	4.9603	-1.2195
C	0.8616	0.9018	0.0014	C	-2.2958	-1.0234	0.4848	H	-4.4471	2.6817	-1.6659
C	1.3562	2.2154	0.2292	C	-3.0859	-0.1372	1.2853	H	-2.6914	0.8659	1.4940
C	0.4892	3.3201	0.1097	C	-4.2865	-0.5285	1.7942	H	-3.0691	0.6863	-1.1786
C	-0.5416	0.7109	-0.1555	C	-4.7964	-1.8291	1.5271	H	-4.8752	0.1513	2.4190
C	3.5657	1.3106	0.6411	C	-4.0641	-2.7128	0.7969	H	-5.7766	-2.1066	1.9281
C	3.1060	-0.0033	0.3061	H	-0.2709	-4.9049	-1.6809	H	-4.4359	-3.7244	0.5977
C	4.0541	-1.0759	0.4401	H	2.0830	-4.3188	-2.2504				

Table 3.570: Table of thermodynamic data as a function of temperature for Tribenzo[*a,f,j*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-59.216	646.173	646.173	∞
100	128.476	368.311	884.842	-51.653	675.444	732.314	-382.513
200	258.703	495.396	658.273	-32.575	659.844	795.431	-207.741
250	333.172	561.071	632.232	-17.790	652.593	830.167	-173.450
298.15	405.576	625.961	625.961	0.000	646.173	864.967	-151.535
300	408.322	628.479	625.969	0.753	645.937	866.323	-150.837
350	480.470	696.897	631.208	22.991	640.062	903.532	-134.842
400	547.297	765.484	643.708	48.710	635.004	941.515	-122.947
450	607.770	833.502	661.026	77.614	630.663	980.095	-113.764
500	661.769	900.387	681.629	109.379	626.934	1019.149	-106.468
600	752.183	1029.364	728.934	180.258	620.956	1098.187	-95.604
700	823.545	1150.884	780.625	259.181	616.701	1178.092	-87.908
800	880.679	1264.719	834.101	344.494	613.965	1258.482	-82.169
900	927.172	1371.222	887.929	434.964	612.549	1339.126	-77.719
1000	965.534	1470.958	941.299	529.658	612.271	1419.882	-74.165
1100	997.538	1564.529	993.748	627.859	612.913	1500.630	-71.257
1200	1024.476	1652.514	1045.016	728.998	614.318	1581.263	-68.829
1300	1047.315	1735.442	1094.967	832.618	616.281	1661.769	-66.769
1400	1066.806	1813.788	1143.539	938.349	618.656	1742.112	-64.998
1500	1083.536	1887.975	1190.717	1045.887	621.354	1822.276	-63.456
1600	1097.974	1958.377	1236.515	1154.980	624.228	1902.242	-62.101
1700	1110.499	2025.326	1280.963	1265.418	627.196	1981.997	-60.898
1800	1121.417	2089.117	1324.102	1377.026	630.174	2061.652	-59.826
1900	1130.980	2150.010	1365.981	1489.657	633.129	2141.080	-58.861
2000	1139.391	2208.240	1406.649	1603.184	635.998	2220.385	-57.989
2100	1146.822	2264.015	1446.157	1717.502	638.694	2299.534	-57.197
2200	1153.413	2317.520	1484.557	1832.520	641.217	2378.561	-56.473
2300	1159.282	2368.924	1521.897	1948.161	643.563	2457.477	-55.810
2400	1164.526	2418.375	1558.227	2064.356	645.649	2536.239	-55.199
2500	1169.230	2466.010	1593.591	2181.048	647.491	2615.053	-54.637
2600	1173.461	2511.952	1628.034	2298.186	649.047	2693.661	-54.115
2700	1177.281	2556.312	1661.598	2415.726	650.323	2772.300	-53.632
2800	1180.739	2599.190	1694.322	2533.630	651.290	2850.922	-53.183
2900	1183.878	2640.680	1726.244	2651.864	651.914	2929.453	-52.764
3000	1186.736	2680.864	1757.398	2770.396	652.246	3007.999	-52.373
3100	1189.344	2719.820	1787.819	2889.202	652.195	3086.449	-52.005
3200	1191.731	2757.618	1817.538	3008.258	651.813	3164.993	-51.662
3300	1193.920	2794.324	1846.584	3127.542	651.077	3243.601	-51.341
3400	1195.931	2829.996	1874.986	3247.036	649.955	3322.134	-51.037
3500	1197.785	2864.690	1902.769	3366.723	648.453	3400.684	-50.751
3600	1199.495	2898.457	1929.961	3486.588	646.597	3479.386	-50.484
3700	1201.077	2931.344	1956.583	3606.618	644.351	3558.163	-50.231
3800	1202.542	2963.394	1982.658	3726.800	641.684	3636.937	-49.992
3900	1203.903	2994.649	2008.207	3847.123	638.644	3715.725	-49.766
4000	1205.168	3025.145	2033.251	3967.577	635.212	3794.760	-49.553
4100	1206.345	3054.919	2057.808	4088.153	631.347	3873.797	-49.352
4200	1207.444	3084.002	2081.896	4208.844	627.083	3952.925	-49.161
4300	1208.470	3112.426	2105.533	4329.640	622.401	4032.052	-48.979
4400	1209.431	3140.219	2128.734	4450.535	617.313	4111.402	-48.808
4500	1210.330	3167.409	2151.514	4571.524	611.837	4190.936	-48.646
4600	1211.174	3194.020	2173.889	4692.600	605.911	4270.608	-48.493
4700	1211.966	3220.076	2195.872	4813.757	599.552	4350.279	-48.347
4800	1212.711	3245.600	2217.477	4934.991	592.815	4430.214	-48.210
4900	1213.413	3270.612	2238.715	5056.298	585.614	4510.135	-48.078
5000	1214.074	3295.133	2259.599	5177.672	578.057	4590.426	-47.955

3.571. Tetrabenzo[*a,c,hi,mn*]naphthacene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 109587-16-8
Point Group: C_{2v}

Length: 15.36 Å
Width: 11.65 Å
Breadth: 3.885 Å
L/B Ratio: 1.318

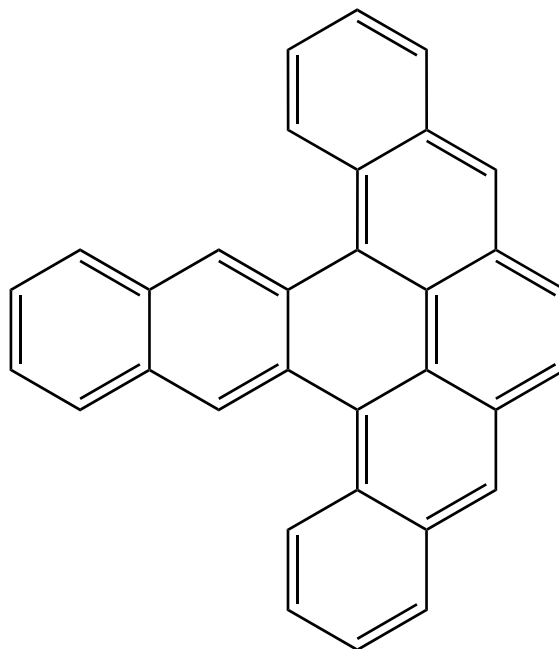
Cartesian coordinates:

C	-4.5458	2.8198	0.0000	C	0.3772	1.3843	0.0000	H	-3.3521	4.6094	0.0000
C	-2.1348	2.8295	0.0000	C	1.5987	0.7050	0.0000	H	-6.7180	1.2401	0.0000
C	-3.3502	3.5144	0.0000	C	1.5989	-0.7045	0.0000	H	-6.7176	-1.2424	0.0000
C	-4.5445	1.4155	0.0000	C	2.8595	1.4317	0.0000	H	-5.4986	-3.3608	0.0000
C	-5.7785	0.6755	0.0000	C	4.0758	0.7284	0.0000	H	-3.3502	-4.6105	0.0000
C	-5.7783	-0.6775	0.0000	C	5.2834	1.4490	0.0000	H	-1.1841	-3.3872	0.0000
C	-4.5440	-1.4170	0.0000	C	5.2853	2.8301	0.0000	H	0.3754	-2.4913	0.0000
C	-4.5447	-2.8213	0.0000	C	4.0750	3.5295	0.0000	H	0.3747	2.4915	0.0000
C	-3.3489	-3.5155	0.0000	C	2.8798	2.8378	0.0000	H	6.2325	0.8915	0.0000
C	-2.1337	-2.8301	0.0000	C	4.0760	-0.7272	0.0000	H	6.2324	3.3792	0.0000
C	-3.3193	0.7182	0.0000	C	2.8599	-1.4308	0.0000	H	4.0777	4.6243	0.0000
C	-3.3191	-0.7192	0.0000	C	2.8805	-2.8369	0.0000	H	1.9221	3.3807	0.0000
C	-2.1006	-1.4384	0.0000	C	4.0759	-3.5283	0.0000	H	1.9230	-3.3800	0.0000
C	-2.1011	1.4378	0.0000	C	5.2860	-2.8285	0.0000	H	4.0790	-4.6231	0.0000
C	-0.8405	0.7059	0.0000	C	5.2838	-1.4475	0.0000	H	6.2333	-3.3774	0.0000
C	-0.8403	-0.7061	0.0000	H	-5.4998	3.3589	0.0000	H	6.2328	-0.8897	0.0000
C	0.3776	-1.3841	0.0000	H	-1.1854	3.3870	0.0000				

Table 3.571: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,c,hi,mn*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-59.293	502.690	502.690	∞
100	130.547	377.492	890.490	-51.300	532.315	588.266	-307.272
200	256.576	504.496	665.784	-32.258	516.679	650.446	-169.876
250	329.860	569.562	640.003	-17.610	509.290	684.742	-143.066
298.15	401.466	633.796	633.796	0.000	502.690	719.149	-125.989
300	404.188	636.288	633.803	0.745	502.447	720.490	-125.446
350	475.854	704.028	638.990	22.763	496.352	757.326	-113.022
400	542.474	771.983	651.368	48.246	491.057	794.968	-103.810
450	602.934	839.430	668.525	76.908	486.474	833.238	-96.718
500	657.047	905.811	688.945	108.433	482.506	872.008	-91.096
600	747.871	1033.961	735.863	178.859	476.075	950.547	-82.751
700	819.710	1154.852	787.173	257.375	471.412	1030.025	-76.860
800	877.294	1268.204	840.295	342.327	468.316	1110.043	-72.477
900	924.183	1374.333	893.801	432.478	466.581	1190.359	-69.085
1000	962.888	1473.772	946.880	526.892	466.022	1270.819	-66.379
1100	995.186	1567.105	999.066	624.843	466.414	1351.298	-64.166
1200	1022.375	1654.896	1050.097	725.759	467.597	1431.684	-62.318
1300	1045.432	1737.665	1099.834	829.180	469.361	1511.960	-60.750
1400	1065.110	1815.879	1148.212	934.733	471.557	1592.087	-59.400
1500	1082.003	1889.954	1195.215	1042.110	474.094	1672.048	-58.225
1600	1096.584	1960.262	1240.852	1151.057	476.822	1751.820	-57.190
1700	1109.234	2027.131	1285.153	1261.362	479.658	1831.391	-56.271
1800	1120.262	2090.852	1328.158	1372.850	482.515	1910.869	-55.451
1900	1129.921	2151.686	1369.913	1485.369	485.359	1990.127	-54.711
2000	1138.419	2209.864	1410.466	1598.795	488.127	2069.267	-54.043
2100	1145.926	2265.593	1449.869	1713.020	490.729	2148.256	-53.434
2200	1152.585	2319.058	1488.171	1827.952	493.167	2227.127	-52.878
2300	1158.515	2370.426	1525.420	1943.513	495.432	2305.891	-52.367
2400	1163.814	2419.846	1561.665	2059.634	497.444	2384.505	-51.896
2500	1168.566	2467.453	1596.950	2176.257	499.218	2463.173	-51.464
2600	1172.843	2513.370	1631.319	2293.331	500.710	2541.637	-51.061
2700	1176.703	2557.707	1664.814	2410.812	501.926	2620.136	-50.689
2800	1180.197	2600.565	1697.472	2528.660	502.837	2698.620	-50.342
2900	1183.370	2642.036	1729.332	2646.841	503.408	2777.014	-50.018
3000	1186.258	2682.203	1760.429	2765.324	503.691	2855.425	-49.716
3100	1188.894	2721.144	1790.795	2884.084	503.594	2933.742	-49.432
3200	1191.307	2758.929	1820.461	3003.096	503.168	3012.155	-49.167
3300	1193.519	2795.622	1849.458	3122.339	502.391	3090.632	-48.920
3400	1195.552	2831.282	1877.814	3241.794	501.230	3169.036	-48.685
3500	1197.425	2865.966	1905.553	3361.444	499.691	3247.458	-48.465
3600	1199.154	2899.723	1932.702	3481.274	497.800	3326.033	-48.258
3700	1200.753	2932.601	1959.284	3601.270	495.521	3404.684	-48.065
3800	1202.235	2964.642	1985.321	3721.421	492.822	3483.333	-47.881
3900	1203.610	2995.889	2010.834	3841.714	489.752	3561.996	-47.707
4000	1204.888	3026.378	2035.843	3962.139	486.292	3640.907	-47.544
4100	1206.079	3056.145	2060.367	4082.688	482.400	3719.822	-47.390
4200	1207.190	3085.222	2084.424	4203.352	478.109	3798.827	-47.244
4300	1208.227	3113.640	2108.030	4324.124	473.402	3877.833	-47.105
4400	1209.198	3141.428	2131.201	4444.996	468.291	3957.061	-46.975
4500	1210.107	3168.612	2153.954	4565.961	462.792	4036.475	-46.853
4600	1210.960	3195.218	2176.302	4687.015	456.844	4116.027	-46.738
4700	1211.761	3221.270	2198.259	4808.152	450.464	4195.578	-46.628
4800	1212.514	3246.790	2219.839	4929.366	443.707	4275.394	-46.525
4900	1213.224	3271.798	2241.053	5050.653	436.486	4355.196	-46.426
5000	1213.892	3296.316	2261.914	5172.009	428.912	4435.368	-46.335

3.572. Anthra[1,2,3,4-*rst*]pentaphene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 31541-07-8
Point Group: C₂

Length: 16.01 Å
Width: 14.10 Å
Breadth: 5.056 Å
L/B Ratio: 1.136

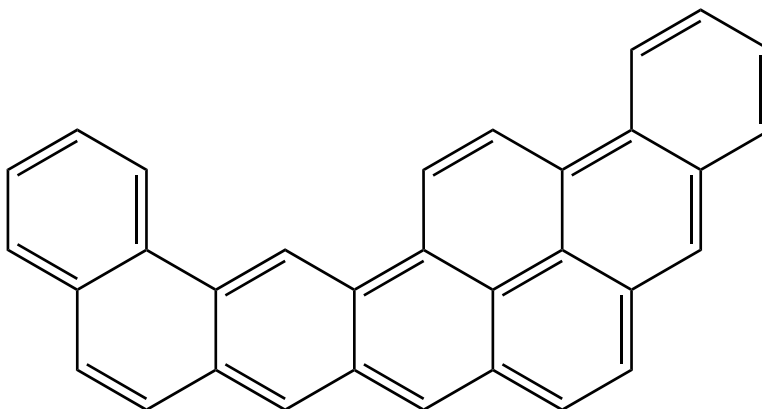
Cartesian coordinates:

C	4.9747	-1.8300	0.1141	C	-1.3172	1.9533	-0.4793	H	2.2164	4.4490	1.0739
C	3.5527	-1.7630	0.1174	C	1.2278	4.4502	0.6014	H	-2.2970	4.4083	-1.0741
C	2.8885	-0.5233	-0.0310	C	0.5879	5.6200	0.3092	H	2.3057	2.0102	0.8772
C	3.7057	0.5997	-0.3483	C	-0.6899	5.6085	-0.3092	H	-2.3424	1.9687	-0.8767
C	5.0703	0.5133	-0.3895	C	-1.3085	4.4273	-0.6017	H	-3.2631	-3.9732	-0.3273
C	5.7217	-0.7107	-0.1202	C	-1.3818	-2.9528	-0.1048	H	3.3355	-3.9123	0.3286
C	1.4546	-0.4782	0.0700	C	-2.7519	-3.0090	-0.2112	H	1.2828	-5.1078	0.1124
C	0.7392	-1.6792	0.0398	C	-3.5199	-1.8282	-0.1163	H	-1.1886	-5.1306	-0.1137
C	1.4357	-2.9269	0.1046	C	-2.8786	-0.5763	0.0310	H	-5.4037	-2.8998	-0.2870
C	2.8066	-2.9577	0.2122	C	-0.6301	-4.1887	-0.0599	H	-6.8009	-0.8785	0.1253
C	-0.7085	-1.6924	-0.0404	C	0.7070	-4.1764	0.0592	H	-5.6977	1.2881	0.6405
C	-1.4459	-0.5047	-0.0707	C	-4.9403	-1.9219	-0.1119	H	-3.2616	1.5025	0.5852
C	-0.7089	0.7521	-0.1459	C	-5.7081	-0.8166	0.1220	H	3.2320	1.5614	-0.5883
C	0.6948	0.7649	0.1448	C	-5.0795	0.4196	0.3895	H	5.6723	1.3928	-0.6413
C	1.2815	1.9768	0.4784	C	-3.7168	0.5315	0.3474	H	6.8155	-0.7521	-0.1227
C	0.6148	3.2016	0.2874	H	-1.1714	6.5634	-0.5440	H	5.4561	-2.7989	0.2902
C	-0.6728	3.1900	-0.2881	H	1.0519	6.5835	0.5442				

Table 3.572: Table of thermodynamic data as a function of temperature for Anthra[1,2,3,4-*rst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-58.963	588.213	588.213	∞
100	127.838	367.380	880.470	-51.309	617.828	674.790	-352.467
200	256.807	493.514	655.392	-32.376	602.083	738.047	-192.754
250	331.121	558.746	629.505	-17.690	594.733	772.888	-161.483
298.15	403.471	623.269	623.269	0.000	588.213	807.809	-141.522
300	406.216	625.774	623.277	0.749	587.973	809.170	-140.886
350	478.371	693.867	628.490	22.882	581.993	846.523	-126.334
400	545.248	762.177	640.933	48.497	576.831	884.664	-115.523
450	605.801	829.958	658.178	77.301	572.389	923.416	-107.185
500	659.898	896.640	678.701	108.970	568.564	962.653	-100.566
600	750.529	1025.295	725.842	179.672	562.410	1042.082	-90.719
700	822.104	1146.576	777.375	258.441	558.000	1122.406	-83.753
800	879.427	1260.231	830.707	343.619	555.130	1203.236	-78.562
900	926.083	1366.597	884.406	433.972	553.597	1284.337	-74.539
1000	964.583	1466.225	937.660	528.565	553.217	1365.560	-71.328
1100	996.703	1559.711	990.005	626.676	553.770	1446.786	-68.701
1200	1023.738	1647.628	1041.181	727.736	555.096	1527.905	-66.507
1300	1046.660	1730.500	1091.049	831.287	556.990	1608.903	-64.645
1400	1066.221	1808.801	1139.546	936.956	559.303	1689.742	-63.044
1500	1083.011	1882.949	1186.657	1044.439	561.946	1770.407	-61.650
1600	1097.502	1953.319	1232.393	1153.482	564.770	1850.877	-60.424
1700	1110.072	2020.241	1276.785	1263.875	567.693	1931.139	-59.335
1800	1121.029	2084.008	1319.873	1375.443	570.631	2011.304	-58.365
1900	1130.626	2144.882	1361.705	1488.036	573.548	2091.244	-57.491
2000	1139.067	2203.094	1402.330	1601.529	576.383	2171.062	-56.701
2100	1146.525	2258.854	1441.798	1715.817	579.048	2250.726	-55.983
2200	1153.139	2312.346	1480.161	1830.806	581.543	2330.271	-55.327
2300	1159.029	2363.737	1517.468	1946.420	583.862	2409.705	-54.725
2400	1164.292	2413.178	1553.765	2062.591	585.924	2488.986	-54.170
2500	1169.012	2460.805	1589.100	2179.261	587.743	2568.319	-53.661
2600	1173.259	2506.738	1623.516	2296.378	589.279	2647.448	-53.187
2700	1177.092	2551.091	1657.054	2413.899	590.535	2726.609	-52.748
2800	1180.562	2593.962	1689.754	2531.784	591.484	2805.754	-52.341
2900	1183.713	2635.446	1721.652	2650.000	592.090	2884.808	-51.960
3000	1186.581	2675.624	1752.785	2768.517	592.406	2963.878	-51.605
3100	1189.198	2714.576	1783.186	2887.308	592.341	3042.852	-51.271
3200	1191.593	2752.369	1812.885	3006.350	591.944	3121.921	-50.959
3300	1193.790	2789.071	1841.913	3125.620	591.195	3201.054	-50.667
3400	1195.809	2824.739	1870.298	3245.102	590.060	3280.112	-50.392
3500	1197.668	2859.430	1898.065	3364.777	588.546	3359.188	-50.132
3600	1199.385	2893.194	1925.241	3484.631	586.679	3438.416	-49.889
3700	1200.972	2926.078	1951.848	3604.649	584.422	3517.720	-49.660
3800	1202.443	2958.125	1977.909	3724.821	581.745	3597.021	-49.443
3900	1203.808	2989.377	2003.445	3845.135	578.695	3676.336	-49.238
4000	1205.078	3019.871	2028.476	3965.580	575.254	3755.898	-49.046
4100	1206.260	3049.642	2053.021	4086.147	571.381	3835.463	-48.863
4200	1207.362	3078.724	2077.098	4206.829	567.108	3915.118	-48.691
4300	1208.392	3107.146	2100.723	4327.617	562.418	3994.774	-48.526
4400	1209.356	3134.937	2123.913	4448.505	557.323	4074.651	-48.371
4500	1210.258	3162.125	2146.684	4569.486	551.839	4154.714	-48.226
4600	1211.105	3188.735	2169.049	4690.555	545.906	4234.914	-48.088
4700	1211.900	3214.790	2191.022	4811.706	539.540	4315.114	-47.956
4800	1212.648	3240.312	2212.618	4932.933	532.797	4395.577	-47.833
4900	1213.352	3265.323	2233.847	5054.234	525.589	4476.027	-47.714
5000	1214.016	3289.843	2254.723	5175.602	518.027	4556.847	-47.604

3.573. Dibenzo[*q,vwx*]hexaphene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 119000-39-4
Point Group: C_s

Length: 18.46 Å
Width: 10.96 Å
Breadth: 3.890 Å
L/B Ratio: 1.685

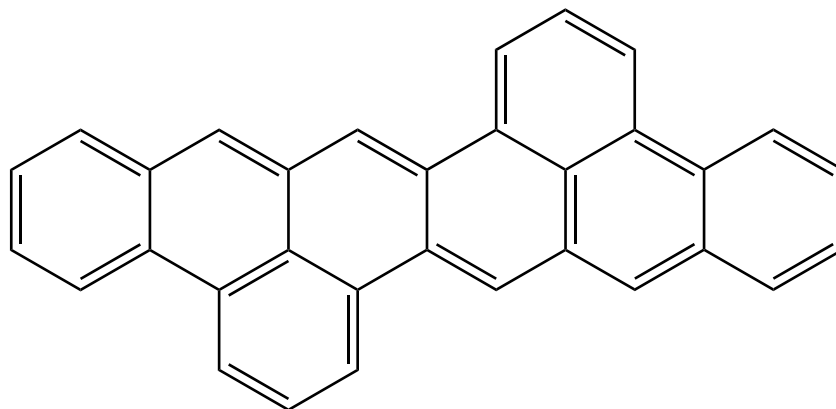
Cartesian coordinates:

C	6.7263	-2.6395	0.0000	C	-3.4391	2.9410	0.0000	H	3.3100	-2.6332	0.0000
C	6.9552	-1.2791	0.0000	C	-3.7765	1.5297	0.0000	H	5.2428	-4.2144	0.0000
C	4.3462	-2.2613	0.0000	C	-5.0807	1.1119	0.0000	H	7.1465	1.3963	0.0000
C	5.4145	-3.1331	0.0000	C	-0.3139	0.0711	0.0000	H	5.2544	3.0010	0.0000
C	4.5583	-0.8694	0.0000	C	-1.3528	1.0073	0.0000	H	2.8596	3.4401	0.0000
C	5.8744	-0.3768	0.0000	C	-2.7095	0.5671	0.0000	H	1.9181	-1.4669	0.0000
C	6.1079	1.0458	0.0000	C	-3.0008	-0.8033	0.0000	H	0.4748	3.9191	0.0000
C	5.0780	1.9191	0.0000	C	-1.9287	-1.7373	0.0000	H	-1.9145	4.4261	0.0000
C	3.4455	0.0629	0.0000	C	-0.6309	-1.3148	0.0000	H	-4.2675	3.6591	0.0000
C	3.7112	1.4574	0.0000	C	-4.3721	-1.2385	0.0000	H	-5.9007	1.8408	0.0000
C	2.6546	2.3622	0.0000	C	-5.4015	-0.2778	0.0000	H	-2.1787	-2.8095	0.0000
C	2.1271	-0.3797	0.0000	C	-6.7527	-0.7046	0.0000	H	0.2021	-2.0347	0.0000
C	1.0562	0.5233	0.0000	C	-7.0583	-2.0426	0.0000	H	-7.5482	0.0493	0.0000
C	1.3253	1.9133	0.0000	C	-6.0294	-3.0054	0.0000	H	-8.1020	-2.3734	0.0000
C	0.2415	2.8470	0.0000	C	-4.7146	-2.6121	0.0000	H	-6.2894	-4.0690	0.0000
C	-1.0558	2.4165	0.0000	H	7.5676	-3.3401	0.0000	H	-3.8989	-3.3514	0.0000
C	-2.1605	3.3577	0.0000	H	7.9796	-0.8895	0.0000				

Table 3.573: Table of thermodynamic data as a function of temperature for Dibenz[*q,vwx*]hexaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.016	511.266	511.266	∞
100	128.364	381.712	893.414	-51.170	541.020	596.549	-311.599
200	256.113	507.734	669.032	-32.259	525.253	658.372	-171.946
250	329.937	572.761	643.242	-17.620	517.856	692.508	-144.689
298.15	401.764	637.031	637.031	0.000	511.266	726.760	-127.323
300	404.490	639.525	637.039	0.746	511.023	728.095	-126.770
350	476.179	707.315	642.229	22.780	504.944	764.768	-114.133
400	542.730	775.310	654.616	48.277	499.664	802.245	-104.760
450	603.101	842.782	671.783	76.950	495.092	840.347	-97.543
500	657.135	909.176	692.213	108.482	491.130	878.950	-91.821
600	747.877	1037.334	739.148	178.911	484.702	957.152	-83.326
700	819.716	1158.224	790.471	257.427	480.040	1036.292	-77.327
800	877.342	1271.580	843.603	342.382	476.946	1115.973	-72.864
900	924.285	1377.718	897.117	432.541	475.219	1195.951	-69.410
1000	963.040	1477.170	950.203	526.967	474.673	1276.071	-66.654
1100	995.377	1570.519	1002.396	624.935	475.082	1356.210	-64.400
1200	1022.594	1658.328	1053.435	725.872	476.285	1436.254	-62.517
1300	1045.668	1741.116	1103.180	829.316	478.072	1516.185	-60.920
1400	1065.355	1819.347	1151.567	934.893	480.293	1595.967	-59.545
1500	1082.251	1893.440	1198.577	1042.294	482.855	1675.580	-58.348
1600	1096.831	1963.764	1244.222	1151.266	485.607	1755.003	-57.294
1700	1109.475	2030.647	1288.531	1261.596	488.467	1834.223	-56.358
1800	1120.497	2094.382	1331.544	1373.107	491.348	1913.349	-55.523
1900	1130.147	2155.228	1373.307	1485.650	494.215	1992.253	-54.770
2000	1138.636	2213.418	1413.869	1599.098	497.005	2071.038	-54.089
2100	1146.133	2269.157	1453.279	1713.344	499.629	2149.671	-53.469
2200	1152.783	2322.632	1491.588	1828.296	502.086	2228.185	-52.903
2300	1158.703	2374.008	1528.844	1943.876	504.371	2306.592	-52.383
2400	1163.993	2423.436	1565.096	2060.016	506.402	2384.847	-51.904
2500	1168.737	2471.050	1600.387	2176.657	508.193	2463.155	-51.464
2600	1173.005	2516.973	1634.763	2293.748	509.702	2541.260	-51.053
2700	1176.857	2561.316	1668.263	2411.244	510.934	2619.398	-50.674
2800	1180.343	2604.180	1700.928	2529.107	511.860	2697.520	-50.322
2900	1183.509	2645.656	1732.793	2647.302	512.445	2775.553	-49.992
3000	1186.391	2685.828	1763.895	2765.799	512.741	2853.602	-49.685
3100	1189.020	2724.773	1794.266	2884.572	512.658	2931.556	-49.395
3200	1191.427	2762.561	1823.938	3003.596	512.244	3009.605	-49.126
3300	1193.633	2799.258	1852.940	3122.850	511.478	3087.719	-48.874
3400	1195.661	2834.922	1881.299	3242.316	510.328	3165.759	-48.635
3500	1197.530	2869.609	1909.044	3361.977	508.800	3243.817	-48.410
3600	1199.254	2903.368	1936.197	3481.817	506.920	3322.028	-48.200
3700	1200.848	2936.249	1962.783	3601.824	504.650	3400.315	-48.003
3800	1202.326	2968.293	1988.824	3721.983	501.960	3478.598	-47.816
3900	1203.697	2999.542	2014.341	3842.285	498.899	3556.896	-47.638
4000	1204.972	3030.033	2039.354	3962.719	495.447	3635.442	-47.473
4100	1206.159	3059.802	2063.881	4083.277	491.564	3713.991	-47.316
4200	1207.266	3088.881	2087.941	4203.949	487.281	3792.630	-47.167
4300	1208.301	3117.301	2111.550	4324.727	482.582	3871.270	-47.026
4400	1209.268	3145.090	2134.725	4445.606	477.478	3950.132	-46.893
4500	1210.175	3172.276	2157.481	4566.579	471.985	4029.180	-46.769
4600	1211.025	3198.884	2179.832	4687.640	466.044	4108.365	-46.651
4700	1211.824	3224.937	2201.792	4808.782	459.670	4187.550	-46.538
4800	1212.575	3250.458	2223.374	4930.003	452.920	4266.999	-46.433
4900	1213.282	3275.468	2244.591	5051.296	445.705	4346.434	-46.333
5000	1213.948	3299.986	2265.455	5172.658	438.136	4426.239	-46.240

3.574. Dibenzo[fg,st]hexacene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 313-97-3
Point Group: C_{2h}

Length: 19.12 Å
Width: 10.22 Å
Breadth: 3.889 Å
L/B Ratio: 1.870

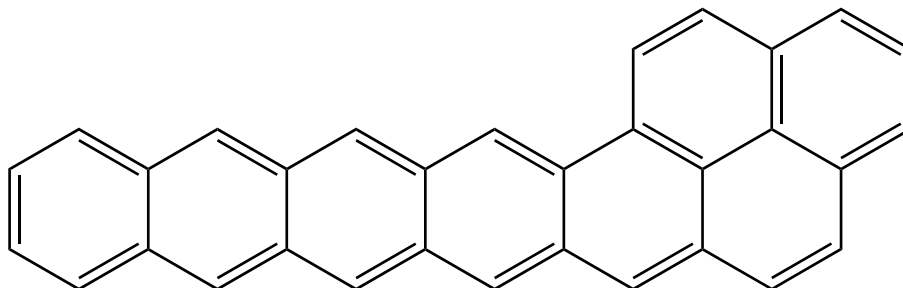
Cartesian coordinates:

C	-7.2365	1.3770	0.0000	C	6.2804	0.8368	0.0000	H	-6.3832	-1.9326	0.0000
C	-7.3876	-0.0206	0.0000	C	-2.5284	-0.5325	0.0000	H	-5.8564	3.0258	0.0000
C	-6.2804	-0.8366	0.0000	C	-3.8040	-1.1252	0.0000	H	-3.4356	2.7859	0.0000
C	-5.9804	1.9369	0.0000	C	-3.9116	-2.5316	0.0000	H	1.0065	-2.5852	0.0000
C	-4.8315	1.1133	0.0000	C	-2.7819	-3.3180	0.0000	H	3.4358	-2.7860	0.0000
C	-4.9805	-0.2853	0.0000	C	-1.5118	-2.7288	0.0000	H	5.8568	-3.0256	0.0000
C	-3.5230	1.6923	0.0000	C	-1.3681	-1.3485	0.0000	H	8.1268	-2.0141	0.0000
C	-2.4080	0.9026	0.0000	C	-1.0836	1.4850	0.0000	H	8.3930	0.4545	0.0000
C	-0.0403	-0.7296	0.0000	C	0.0403	0.7293	0.0000	H	6.3830	1.9329	0.0000
C	1.0837	-1.4852	0.0000	C	1.3681	1.3483	0.0000	H	-4.9166	-2.9807	0.0000
C	2.4080	-0.9027	0.0000	C	2.5284	0.5324	0.0000	H	-2.8688	-4.4095	0.0000
C	3.5231	-1.6923	0.0000	C	3.8039	1.1252	0.0000	H	-0.6125	-3.3639	0.0000
C	4.9805	0.2854	0.0000	C	3.9115	2.5316	0.0000	H	-1.0062	2.5850	0.0000
C	4.8316	-1.1132	0.0000	C	2.7816	3.3179	0.0000	H	4.9164	2.9809	0.0000
C	5.9806	-1.9367	0.0000	C	1.5117	2.7286	0.0000	H	2.8686	4.4094	0.0000
C	7.2366	-1.3766	0.0000	H	-8.1266	2.0145	0.0000	H	0.6125	3.3637	0.0000
C	7.3876	0.0210	0.0000	H	-8.3931	-0.4540	0.0000				

Table 3.574: Table of thermodynamic data as a function of temperature for Dibenzo[fg,st]hexacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-59.641	553.250	553.250	∞
100	131.417	382.062	897.934	-51.587	582.586	638.081	-333.292
200	258.076	509.927	672.014	-32.418	567.078	699.759	-182.755
250	331.504	575.344	646.108	-17.691	559.768	733.775	-153.311
298.15	403.169	639.874	639.874	0.000	553.250	767.896	-134.529
300	405.891	642.376	639.882	0.748	553.009	769.226	-133.931
350	477.527	710.378	645.088	22.851	546.999	805.751	-120.249
400	544.058	778.551	657.513	48.415	541.786	843.070	-110.091
450	604.404	846.179	674.726	77.154	537.279	881.006	-102.262
500	658.398	912.708	695.209	108.750	533.381	919.436	-96.051
600	749.012	1041.085	742.252	179.300	527.074	997.273	-86.819
700	820.692	1162.139	793.680	257.921	522.518	1076.030	-80.293
800	878.161	1275.615	846.908	342.966	519.513	1155.313	-75.433
900	924.963	1381.840	900.508	433.199	517.861	1234.882	-71.669
1000	963.598	1481.357	953.670	527.687	517.377	1314.587	-68.666
1100	995.836	1574.755	1005.932	625.706	517.837	1394.304	-66.209
1200	1022.974	1662.601	1057.030	726.685	519.081	1473.923	-64.157
1300	1045.984	1745.416	1106.829	830.163	520.903	1553.426	-62.416
1400	1065.620	1823.669	1155.263	935.769	523.153	1632.776	-60.918
1500	1082.474	1897.778	1202.315	1043.195	525.738	1711.956	-59.614
1600	1097.019	1968.115	1247.999	1152.187	528.512	1790.945	-58.467
1700	1109.637	2035.009	1292.342	1262.534	531.389	1869.729	-57.449
1800	1120.636	2098.753	1335.386	1374.060	534.285	1948.418	-56.540
1900	1130.268	2159.606	1377.177	1486.616	537.165	2026.884	-55.722
2000	1138.741	2217.801	1417.764	1600.075	539.966	2105.232	-54.982
2100	1146.226	2273.545	1457.197	1714.331	542.600	2183.426	-54.309
2200	1152.865	2327.024	1495.528	1829.292	545.066	2261.501	-53.694
2300	1158.776	2378.404	1532.804	1944.880	547.359	2339.468	-53.130
2400	1164.058	2427.835	1569.074	2061.027	549.396	2417.283	-52.610
2500	1168.795	2475.452	1604.382	2177.674	551.193	2495.152	-52.132
2600	1173.058	2521.377	1638.773	2294.770	552.708	2572.816	-51.687
2700	1176.904	2565.722	1672.288	2412.271	553.945	2650.514	-51.276
2800	1180.387	2608.587	1704.966	2530.139	554.875	2728.195	-50.894
2900	1183.549	2650.065	1736.845	2648.338	555.465	2805.787	-50.537
3000	1186.427	2690.238	1767.958	2766.839	555.765	2883.396	-50.203
3100	1189.054	2729.184	1798.341	2885.615	555.685	2960.909	-49.890
3200	1191.458	2766.974	1828.023	3004.642	555.274	3038.517	-49.598
3300	1193.662	2803.671	1857.035	3123.900	554.512	3116.189	-49.324
3400	1195.688	2839.336	1885.404	3243.369	553.365	3193.788	-49.066
3500	1197.554	2874.023	1913.157	3363.032	551.839	3271.405	-48.822
3600	1199.277	2907.784	1940.319	3482.875	549.961	3349.173	-48.594
3700	1200.870	2940.665	1966.913	3602.883	547.693	3427.019	-48.380
3800	1202.346	2972.710	1992.961	3723.045	545.006	3504.861	-48.177
3900	1203.716	3003.959	2018.485	3843.349	541.947	3582.717	-47.984
4000	1204.990	3034.451	2043.505	3963.785	538.497	3660.821	-47.804
4100	1206.176	3064.220	2068.039	4084.344	534.615	3738.929	-47.634
4200	1207.282	3093.299	2092.105	4205.017	530.333	3817.126	-47.472
4300	1208.316	3121.720	2115.720	4325.798	525.636	3895.324	-47.318
4400	1209.283	3149.509	2138.901	4446.678	520.533	3973.744	-47.173
4500	1210.188	3176.696	2161.662	4567.652	515.042	4052.350	-47.037
4600	1211.038	3203.304	2184.018	4688.714	509.102	4131.093	-46.909
4700	1211.836	3229.357	2205.983	4809.858	502.730	4209.836	-46.786
4800	1212.586	3254.878	2227.570	4931.080	495.980	4288.843	-46.671
4900	1213.293	3279.888	2248.792	5052.374	488.767	4367.836	-46.561
5000	1213.959	3304.407	2269.659	5173.737	481.199	4447.199	-46.459

3.575. Naphtho[2,1,8-*yz*a]hexacene



Formula: $C_{32}H_{18}$
Mass: 402.485 g/mol
CAS Number: 196-46-3
Point Group: C_s

Length: 20.75 Å
Width: 9.641 Å
Breadth: 3.885 Å
L/B Ratio: 2.152

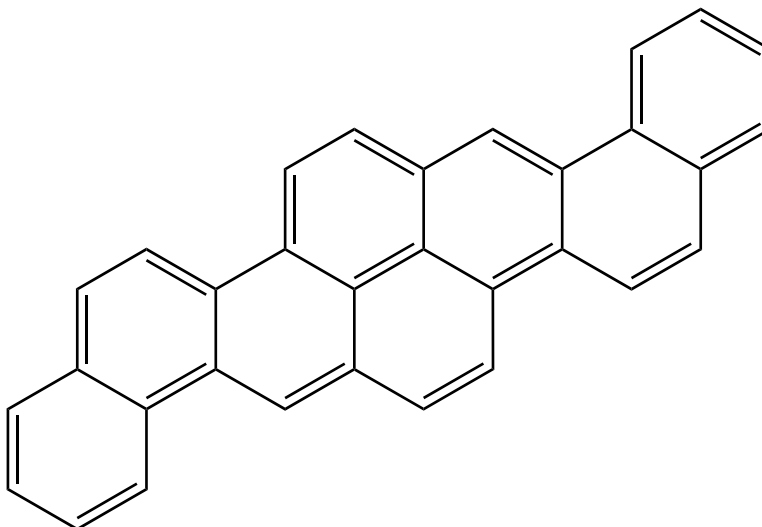
Cartesian coordinates:

C	8.4454	-1.1843	0.0000	C	-1.0572	1.3568	0.0000	H	7.6488	2.1496	0.0000
C	8.6102	0.2397	0.0000	C	-2.2208	2.2035	0.0000	H	7.0731	-2.8241	0.0000
C	7.5329	1.0598	0.0000	C	-3.4766	1.6770	0.0000	H	5.2097	2.4323	0.0000
C	7.2092	-1.7366	0.0000	C	-4.6534	2.5272	0.0000	H	4.6340	-2.5422	0.0000
C	6.0307	-0.9058	0.0000	C	-5.8962	2.0119	0.0000	H	2.7755	2.7127	0.0000
C	6.1957	0.5202	0.0000	C	-6.1183	0.5792	0.0000	H	2.1998	-2.2591	0.0000
C	5.0894	1.3418	0.0000	C	-7.3952	0.0454	0.0000	H	0.3400	2.9922	0.0000
C	4.7659	-1.4530	0.0000	C	-7.5818	-1.3464	0.0000	H	-0.2443	-1.9794	0.0000
C	3.6146	-0.6223	0.0000	C	-6.5026	-2.2001	0.0000	H	-2.0690	3.2903	0.0000
C	3.7787	0.7959	0.0000	C	-4.9915	-0.2887	0.0000	H	-4.4922	3.6117	0.0000
C	2.6489	1.6229	0.0000	C	-5.1870	-1.6844	0.0000	H	-6.7790	2.6617	0.0000
C	2.3256	-1.1693	0.0000	C	-4.0479	-2.5437	0.0000	H	-8.2683	0.7076	0.0000
C	1.1997	-0.3429	0.0000	C	-2.7886	-2.0239	0.0000	H	-8.6006	-1.7481	0.0000
C	1.3636	1.0756	0.0000	C	-2.5706	-0.6146	0.0000	H	-6.6502	-3.2860	0.0000
C	0.2076	1.9029	0.0000	C	-3.6650	0.2432	0.0000	H	-4.2078	-3.6279	0.0000
C	-0.1144	-0.8849	0.0000	H	9.3429	-1.8113	0.0000	H	-1.9037	-2.6791	0.0000
C	-1.2244	-0.0716	0.0000	H	9.6272	0.6451	0.0000				

Table 3.575: Table of thermodynamic data as a function of temperature for Naphtho[2,1,8-*yz*]hexacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-59.546	563.005	563.005	∞
100	128.714	386.916	903.063	-51.615	592.315	647.324	-338.120
200	258.434	513.715	676.617	-32.580	576.671	708.594	-185.062
250	333.274	579.374	650.568	-17.799	569.417	742.415	-155.116
298.15	405.780	644.295	644.295	0.000	563.005	776.333	-136.008
300	408.526	646.813	644.302	0.753	562.770	777.655	-135.399
350	480.589	715.258	649.543	23.000	556.903	813.947	-121.473
400	547.262	783.851	662.047	48.722	551.848	851.012	-111.128
450	607.586	851.856	679.367	77.620	547.501	888.673	-103.152
500	661.472	918.716	699.971	109.373	543.760	926.811	-96.821
600	751.785	1047.627	747.268	180.215	537.746	1004.019	-87.406
700	823.167	1169.086	798.944	259.099	533.452	1082.101	-80.746
800	880.378	1282.875	852.402	344.378	530.681	1160.673	-75.783
900	926.962	1389.348	906.213	434.822	529.239	1239.504	-71.937
1000	965.409	1489.066	959.566	529.500	528.945	1318.447	-68.867
1100	997.485	1582.629	1012.000	627.692	529.578	1397.385	-66.355
1200	1024.478	1670.611	1063.255	728.828	530.980	1476.209	-64.256
1300	1047.359	1753.542	1113.195	832.450	532.946	1554.905	-62.476
1400	1066.879	1831.892	1161.758	938.188	535.327	1633.437	-60.943
1500	1083.630	1906.085	1208.929	1045.734	538.033	1711.791	-59.609
1600	1098.082	1976.494	1254.720	1154.837	540.917	1789.945	-58.435
1700	1110.615	2043.449	1299.163	1265.286	543.897	1867.889	-57.392
1800	1121.538	2107.246	1342.299	1376.906	546.887	1945.731	-56.462
1900	1131.102	2168.147	1384.174	1489.549	549.853	2023.345	-55.624
2000	1139.514	2226.383	1424.839	1603.088	552.735	2100.837	-54.867
2100	1146.943	2282.164	1464.345	1717.419	555.443	2178.171	-54.178
2200	1153.531	2335.675	1502.743	1832.449	557.978	2255.383	-53.548
2300	1159.397	2387.083	1540.083	1948.101	560.336	2332.483	-52.971
2400	1164.638	2436.539	1576.411	2064.308	562.433	2409.429	-52.439
2500	1169.337	2484.179	1611.775	2181.011	564.286	2486.426	-51.950
2600	1173.565	2530.125	1646.218	2298.159	565.853	2563.217	-51.495
2700	1177.380	2574.489	1679.781	2415.710	567.139	2640.038	-51.074
2800	1180.834	2617.371	1712.505	2533.623	568.116	2716.843	-50.682
2900	1183.970	2658.863	1744.427	2651.866	568.748	2793.555	-50.316
3000	1186.824	2699.050	1775.581	2770.408	569.089	2870.283	-49.975
3100	1189.428	2738.009	1806.002	2889.222	569.048	2946.914	-49.654
3200	1191.811	2775.810	1835.721	3008.286	568.674	3023.639	-49.355
3300	1193.997	2812.518	1864.767	3127.578	567.946	3100.428	-49.075
3400	1196.005	2848.193	1893.169	3247.080	566.831	3177.141	-48.810
3500	1197.855	2882.889	1920.954	3366.774	565.336	3253.872	-48.560
3600	1199.563	2916.658	1948.145	3486.646	563.487	3330.753	-48.327
3700	1201.142	2949.547	1974.768	3606.682	561.248	3407.711	-48.107
3800	1202.605	2981.599	2000.843	3726.871	558.587	3484.664	-47.899
3900	1203.963	3012.855	2026.393	3847.200	555.553	3561.632	-47.702
4000	1205.225	3043.352	2051.437	3967.660	552.127	3638.846	-47.517
4100	1206.401	3073.127	2075.995	4088.242	548.268	3716.063	-47.342
4200	1207.497	3102.212	2100.084	4208.937	544.009	3793.369	-47.176
4300	1208.522	3130.637	2123.721	4329.739	539.332	3870.676	-47.018
4400	1209.480	3158.431	2146.922	4450.640	534.250	3948.204	-46.870
4500	1210.377	3185.622	2169.704	4571.633	528.778	4025.917	-46.731
4600	1211.219	3212.234	2192.079	4692.713	522.857	4103.767	-46.599
4700	1212.010	3238.291	2214.063	4813.875	516.502	4181.617	-46.473
4800	1212.754	3263.816	2235.668	4935.114	509.770	4259.730	-46.354
4900	1213.454	3288.830	2256.906	5056.424	502.573	4337.829	-46.241
5000	1214.114	3313.351	2277.791	5177.803	495.020	4416.299	-46.136

3.576. Benzo[*tuv*]naphtho[2,1-*b*]picene



Formula: C₃₂H₁₈
Mass: 402.485 g/mol
CAS Number: 119123-35-2
Point Group: C_{2h}

Length: 20.16 Å
Width: 9.195 Å
Breadth: 3.885 Å
L/B Ratio: 2.192

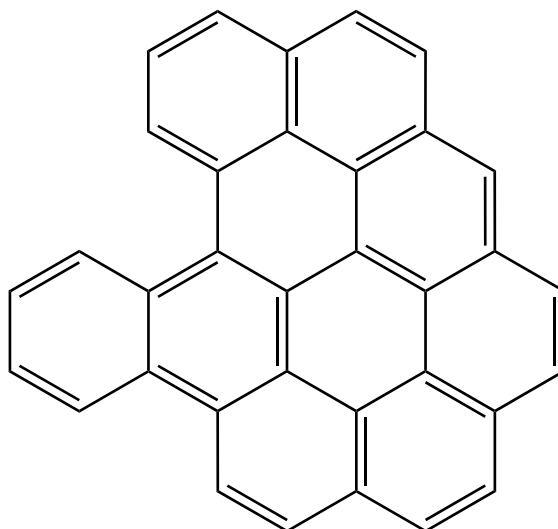
Cartesian coordinates:

C	2.7187	1.4187	0.0000	C	2.9187	-1.0089	0.0000	H	1.4826	-3.2968	0.0000
C	1.5051	-1.1180	0.0000	C	3.7539	-2.1788	0.0000	H	-3.2089	-2.4056	0.0000
C	-0.5023	-2.5001	0.0000	C	5.1035	-2.0821	0.0000	H	0.9946	3.4795	0.0000
C	0.8456	-2.3990	0.0000	C	-4.9670	-0.3709	0.0000	H	-1.4826	3.2969	0.0000
C	-1.3349	-1.3243	0.0000	C	-5.7473	0.7981	0.0000	H	-3.2554	3.1603	0.0000
C	-2.7187	-1.4186	0.0000	C	-7.1549	0.7006	0.0000	H	-5.7338	2.9789	0.0000
C	0.7162	0.0460	0.0000	C	-7.7657	-0.5332	0.0000	H	3.2552	-3.1602	0.0000
C	1.3349	1.3244	0.0000	C	-6.9899	-1.7036	0.0000	H	5.7337	-2.9790	0.0000
C	0.5023	2.5002	0.0000	C	-5.6157	-1.6242	0.0000	H	-7.7544	1.6180	0.0000
C	-0.8456	2.3991	0.0000	C	4.9670	0.3709	0.0000	H	-8.8578	-0.6099	0.0000
C	-1.5051	1.1181	0.0000	C	5.7473	-0.7982	0.0000	H	-7.4858	-2.6797	0.0000
C	-0.7162	-0.0459	0.0000	C	7.1549	-0.7007	0.0000	H	-4.9980	-2.5353	0.0000
C	-3.5215	-0.2660	0.0000	C	7.7657	0.5331	0.0000	H	7.7544	-1.6182	0.0000
C	-2.9187	1.0090	0.0000	C	6.9899	1.7035	0.0000	H	8.8579	0.6098	0.0000
C	-3.7540	2.1789	0.0000	C	5.6158	1.6242	0.0000	H	7.4860	2.6796	0.0000
C	-5.1036	2.0821	0.0000	H	3.2089	2.4057	0.0000	H	4.9981	2.5353	0.0000
C	3.5215	0.2661	0.0000	H	-0.9945	-3.4794	0.0000				

Table 3.576: Table of thermodynamic data as a function of temperature for Benzo[*tu*v]naphtho[2,1-*b*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.095	509.663	509.663	∞
100	129.239	375.180	887.322	-51.214	539.373	595.556	-311.080
200	256.248	501.575	662.846	-32.254	523.655	658.007	-171.850
250	329.864	566.607	637.063	-17.614	516.259	692.450	-144.676
298.15	401.587	630.855	630.855	0.000	509.663	726.998	-127.364
300	404.310	633.347	630.862	0.745	509.420	728.345	-126.814
350	475.957	701.106	636.050	22.770	503.331	765.328	-114.217
400	542.500	769.070	648.432	48.255	498.040	803.116	-104.874
450	602.878	836.516	665.591	76.916	493.456	841.531	-97.680
500	656.922	902.887	686.012	108.437	489.483	880.448	-91.978
600	747.672	1031.007	732.929	178.846	483.035	959.280	-83.511
700	819.501	1151.865	784.235	257.342	478.352	1039.055	-77.534
800	877.109	1265.191	837.349	342.274	475.235	1119.374	-73.086
900	924.033	1371.300	890.846	432.408	473.484	1199.992	-69.644
1000	962.773	1470.725	943.916	526.809	472.912	1280.755	-66.898
1100	995.103	1564.048	996.094	624.750	473.294	1361.539	-64.653
1200	1022.318	1651.834	1047.118	725.659	474.469	1442.231	-62.777
1300	1045.396	1734.599	1096.848	829.076	476.229	1522.814	-61.186
1400	1065.090	1812.811	1145.221	934.626	478.423	1603.248	-59.817
1500	1081.996	1886.885	1192.218	1042.001	480.958	1683.515	-58.624
1600	1096.585	1957.193	1237.851	1150.948	483.686	1763.595	-57.574
1700	1109.242	2024.062	1282.148	1261.254	486.522	1843.473	-56.642
1800	1120.275	2087.784	1325.149	1372.742	489.380	1923.258	-55.810
1900	1129.937	2148.618	1366.901	1485.263	492.226	2002.822	-55.060
2000	1138.437	2206.797	1407.452	1598.691	494.995	2082.269	-54.382
2100	1145.946	2262.527	1446.852	1712.918	497.600	2161.564	-53.765
2200	1152.606	2315.993	1485.152	1827.852	500.039	2240.742	-53.201
2300	1158.536	2367.362	1522.399	1943.415	502.307	2319.813	-52.684
2400	1163.836	2416.783	1558.642	2059.538	504.321	2398.733	-52.206
2500	1168.588	2464.391	1593.926	2176.163	506.097	2477.706	-51.768
2600	1172.864	2510.309	1628.293	2293.240	507.591	2556.478	-51.359
2700	1176.724	2554.647	1661.786	2410.722	508.810	2635.282	-50.982
2800	1180.218	2597.505	1694.444	2528.572	509.723	2714.072	-50.631
2900	1183.390	2638.977	1726.303	2646.755	510.296	2792.772	-50.302
3000	1186.278	2679.145	1757.398	2765.241	510.580	2871.489	-49.996
3100	1188.913	2718.087	1787.763	2884.002	510.486	2950.112	-49.708
3200	1191.325	2755.872	1817.429	3003.016	510.061	3028.830	-49.440
3300	1193.537	2792.565	1846.426	3122.261	509.286	3107.613	-49.188
3400	1195.569	2828.226	1874.780	3241.717	508.127	3186.322	-48.951
3500	1197.442	2862.910	1902.519	3361.369	506.590	3265.050	-48.727
3600	1199.170	2896.668	1929.668	3481.201	504.700	3343.931	-48.518
3700	1200.769	2929.546	1956.249	3601.199	502.422	3422.888	-48.322
3800	1202.250	2961.588	1982.286	3721.351	499.725	3501.842	-48.135
3900	1203.624	2992.835	2007.798	3841.645	496.657	3580.810	-47.959
4000	1204.902	3023.325	2032.807	3962.072	493.198	3660.027	-47.794
4100	1206.092	3053.092	2057.330	4082.623	489.307	3739.247	-47.638
4200	1207.203	3082.169	2081.386	4203.288	485.018	3818.557	-47.490
4300	1208.240	3110.588	2104.992	4324.061	480.312	3897.868	-47.349
4400	1209.210	3138.376	2128.163	4444.934	475.202	3977.402	-47.217
4500	1210.119	3165.560	2150.916	4565.901	469.704	4057.121	-47.093
4600	1210.971	3192.167	2173.263	4686.956	463.757	4136.978	-46.976
4700	1211.772	3218.219	2195.220	4808.093	457.379	4216.834	-46.864
4800	1212.525	3243.739	2216.799	4929.309	450.623	4296.955	-46.759
4900	1213.234	3268.748	2238.013	5050.597	443.403	4377.062	-46.659
5000	1213.902	3293.265	2258.874	5171.954	435.829	4457.540	-46.567

3.577. Benzo[*p*]naphtho[8,1,2-*abc*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 75450-00-9
Point Group: C₁

Length: 13.71 Å
Width: 12.95 Å
Breadth: 4.985 Å
L/B Ratio: 1.059

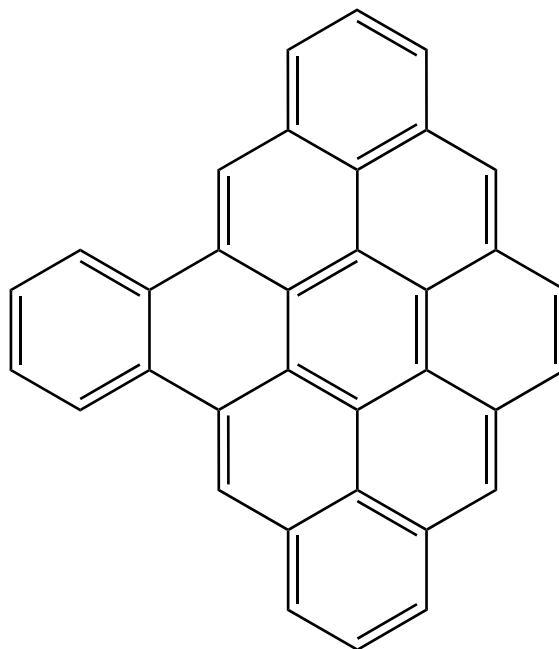
Cartesian coordinates:

C	-0.1920	-1.0606	-0.0522	C	-2.6127	-0.5761	0.0036	H	-0.9968	-4.8801	-0.4278
C	-0.7680	-3.8131	-0.3156	C	0.6231	3.1274	-0.0280	H	-5.2499	-2.7538	-0.1692
C	-1.8220	-2.8849	-0.2317	C	1.6836	2.2071	-0.1656	H	-3.3917	-4.3865	-0.3792
C	-1.5347	-1.5110	-0.0986	C	2.9432	2.7214	-0.5584	H	-1.5872	4.6324	0.3898
C	-4.2055	-2.4219	-0.1517	C	3.1651	4.0707	-0.6952	H	-3.9322	3.8171	0.4962
C	-3.1878	-3.3156	-0.2652	C	2.1290	4.9846	-0.4468	H	-5.5431	1.9746	0.3651
C	0.1174	0.3464	0.0195	C	0.8780	4.5150	-0.1319	H	-6.0300	-0.4491	0.1213
C	1.4383	0.7905	0.0205	C	2.4981	-0.1901	0.2025	H	3.7676	2.0269	-0.7708
C	-0.9749	1.2808	0.0884	C	4.5320	-2.1470	0.4396	H	4.1494	4.4396	-1.0020
C	-0.7257	2.6534	0.1478	C	4.8034	-0.8081	0.6937	H	2.3193	6.0597	-0.5242
C	-1.8129	3.5577	0.3154	C	3.8066	0.1485	0.5801	H	0.0451	5.2159	0.0313
C	-3.1013	3.1138	0.3698	C	3.2285	-2.5383	0.1376	H	5.3311	-2.8945	0.4966
C	-2.3260	0.8161	0.1198	C	2.1996	-1.5682	0.0623	H	5.8148	-0.5046	0.9848
C	-3.3874	1.7259	0.2513	C	0.8448	-2.0026	-0.0978	H	4.0619	1.1952	0.7953
C	-4.7290	1.2487	0.2572	C	0.5482	-3.3878	-0.2374	H	1.3960	-5.3914	-0.4278
C	-4.9968	-0.0833	0.1251	C	1.6377	-4.3348	-0.2647	H	3.7389	-4.6488	-0.0791
C	-3.9379	-1.0243	-0.0076	C	2.9110	-3.9302	-0.0775				

Table 3.577: Table of thermodynamic data as a function of temperature for Benzo[*p*]naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.442	507.407	507.407	∞
100	118.433	359.334	864.274	-50.494	534.351	582.236	-304.122
200	253.189	480.730	641.778	-32.210	519.999	635.870	-166.069
250	329.546	545.387	615.990	-17.651	513.326	665.608	-139.068
298.15	403.364	609.764	609.764	0.000	507.407	695.490	-121.845
300	406.160	612.268	609.772	0.749	507.187	696.655	-121.296
350	479.606	680.451	614.989	22.912	501.744	728.676	-108.747
400	547.681	749.005	627.457	48.619	497.028	761.414	-99.428
450	609.359	817.138	644.754	77.573	492.941	794.713	-92.246
500	664.485	884.250	665.359	109.446	489.386	828.463	-86.547
600	756.780	1013.897	712.739	180.695	483.551	896.856	-78.077
700	829.434	1136.230	764.591	260.147	479.218	966.110	-72.091
800	887.309	1250.905	818.292	346.090	476.223	1035.874	-67.634
900	934.114	1358.211	872.387	437.241	474.392	1105.932	-64.185
1000	972.490	1458.681	926.048	532.633	473.570	1176.155	-61.435
1100	1004.316	1552.908	978.797	631.522	473.550	1246.433	-59.187
1200	1030.961	1641.470	1030.367	733.324	474.195	1316.659	-57.311
1300	1053.449	1724.904	1080.615	837.576	475.312	1386.825	-55.722
1400	1072.563	1803.691	1129.476	943.902	476.766	1456.896	-54.356
1500	1088.914	1878.263	1176.932	1051.996	478.481	1526.857	-53.169
1600	1102.985	1949.000	1222.995	1161.608	480.315	1596.687	-52.125
1700	1115.161	2016.242	1267.695	1272.530	482.197	1666.373	-51.200
1800	1125.753	2080.290	1311.074	1384.588	484.045	1736.025	-50.377
1900	1135.012	2141.409	1353.180	1497.636	485.831	1805.511	-49.636
2000	1143.144	2199.839	1394.063	1611.553	487.501	1874.939	-48.967
2100	1150.318	2255.790	1433.775	1726.233	488.968	1944.271	-48.360
2200	1156.674	2309.453	1472.367	1841.589	490.234	2013.538	-47.806
2300	1162.327	2360.996	1509.890	1957.545	491.299	2082.756	-47.300
2400	1167.374	2410.573	1546.392	2074.034	492.081	2151.870	-46.833
2500	1171.896	2458.321	1581.920	2191.002	492.599	2221.096	-46.406
2600	1175.962	2504.364	1616.519	2308.398	492.811	2290.165	-46.009
2700	1179.630	2548.815	1650.230	2426.181	492.726	2359.324	-45.643
2800	1182.948	2591.777	1683.093	2544.313	492.313	2428.512	-45.304
2900	1185.959	2633.341	1715.148	2662.760	491.541	2497.659	-44.987
3000	1188.699	2673.594	1746.429	2781.495	490.464	2566.872	-44.692
3100	1191.198	2712.612	1776.970	2900.492	488.989	2636.029	-44.416
3200	1193.484	2750.468	1806.803	3019.728	487.168	2705.331	-44.159
3300	1195.580	2787.226	1835.959	3139.183	484.983	2774.747	-43.920
3400	1197.506	2822.947	1864.465	3258.838	482.397	2844.123	-43.694
3500	1199.279	2857.685	1892.349	3378.679	479.419	2913.559	-43.482
3600	1200.915	2891.493	1919.635	3498.689	476.078	2983.200	-43.284
3700	1202.428	2924.418	1946.348	3618.858	472.334	3052.951	-43.099
3800	1203.829	2956.504	1972.511	3739.171	468.160	3122.743	-42.924
3900	1205.130	2987.791	1998.144	3859.620	463.603	3192.578	-42.759
4000	1206.339	3018.317	2023.269	3980.194	458.645	3262.712	-42.606
4100	1207.464	3048.119	2047.903	4100.885	453.244	3332.883	-42.461
4200	1208.514	3077.229	2072.066	4221.684	447.433	3403.180	-42.324
4300	1209.494	3105.677	2095.774	4342.585	441.198	3473.510	-42.194
4400	1210.411	3133.493	2119.043	4463.581	434.548	3544.100	-42.073
4500	1211.270	3160.705	2141.890	4584.666	427.502	3614.913	-41.960
4600	1212.076	3187.336	2164.329	4705.833	419.996	3685.904	-41.854
4700	1212.832	3213.411	2186.373	4827.079	412.050	3756.921	-41.753
4800	1213.544	3238.953	2208.037	4948.398	403.717	3828.243	-41.659
4900	1214.213	3263.982	2229.332	5069.787	394.909	3899.573	-41.569
5000	1214.845	3288.519	2250.271	5191.240	385.740	3971.314	-41.487

3.578. Tribenzo[*a,ef,no*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 128345-68-6
Point Group: C_{2v}

Length: 15.84 Å
Width: 14.15 Å
Breadth: 3.887 Å
L/B Ratio: 1.120

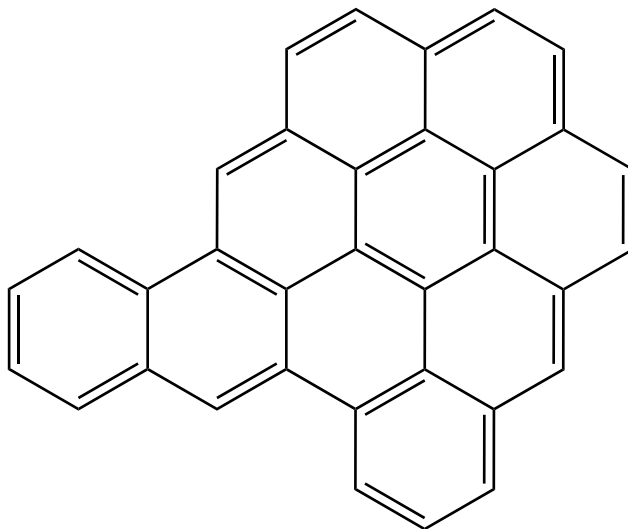
Cartesian coordinates:

C	4.9513	-0.4624	0.0000	C	-4.9633	1.8121	0.0000	H	5.5215	-1.3982	0.0000
C	5.6162	0.7588	0.0000	C	-5.6356	0.5972	0.0000	H	6.7113	0.7777	0.0000
C	4.9092	1.9538	0.0000	C	-4.9360	-0.6044	0.0000	H	5.4455	2.9095	0.0000
C	3.5085	1.9469	0.0000	C	-2.8424	0.6274	0.0000	H	3.3014	4.1173	0.0000
C	2.7543	3.1664	0.0000	C	-3.5374	-0.6047	0.0000	H	1.1607	5.3202	0.0000
C	1.3887	3.1468	0.0000	C	-2.7863	-1.8263	0.0000	H	-1.3129	5.2847	0.0000
C	0.6100	4.3723	0.0000	C	-1.4140	0.6370	0.0000	H	-3.4182	4.0208	0.0000
C	-0.7352	4.3530	0.0000	C	-0.6937	-0.5817	0.0000	H	3.4165	-2.6834	0.0000
C	-1.4785	3.1056	0.0000	C	-1.4210	-1.8298	0.0000	H	-5.5268	2.7520	0.0000
C	-2.8440	3.0861	0.0000	C	1.4730	-1.7882	0.0000	H	-6.7308	0.5847	0.0000
C	-0.7291	1.8725	0.0000	C	0.7101	-0.5615	0.0000	H	-5.4791	-1.5562	0.0000
C	0.6750	1.8927	0.0000	C	0.7471	-3.0582	0.0000	H	-3.3380	-2.7804	0.0000
C	1.3951	0.6774	0.0000	C	-0.6590	-3.0784	0.0000	H	-2.4253	-4.3210	0.0000
C	2.8375	-1.7455	0.0000	C	-1.3244	-4.3119	0.0000	H	-1.1527	-6.4587	0.0000
C	3.5533	-0.5029	0.0000	C	-0.6175	-5.5036	0.0000	H	1.3377	-6.4229	0.0000
C	2.8232	0.7087	0.0000	C	0.7753	-5.4836	0.0000	H	2.5484	-4.2496	0.0000
C	-3.5629	1.8454	0.0000	C	1.4476	-4.2721	0.0000				

Table 3.578: Table of thermodynamic data as a function of temperature for Tribenzo[*a,ef,no*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.582	521.704	521.704	∞
100	119.267	355.809	861.607	-50.580	548.562	596.799	-311.730
200	253.578	477.700	638.835	-32.227	534.279	650.755	-169.956
250	329.710	542.419	613.037	-17.655	527.619	680.643	-142.210
298.15	403.369	606.810	606.810	0.000	521.704	710.668	-124.504
300	406.159	609.314	606.818	0.749	521.485	711.838	-123.939
350	479.474	677.487	612.034	22.908	516.038	744.007	-111.035
400	547.445	746.016	624.500	48.606	511.312	776.894	-101.450
450	609.049	814.117	641.792	77.546	507.212	810.343	-94.060
500	664.127	881.193	662.389	109.402	503.640	844.245	-88.196
600	756.392	1010.771	709.749	180.614	497.767	912.947	-79.477
700	829.067	1133.046	761.577	260.028	493.396	982.517	-73.315
800	886.985	1247.674	815.254	345.936	490.366	1052.601	-68.726
900	933.839	1354.945	869.326	437.058	488.505	1122.984	-65.175
1000	972.260	1455.388	922.964	532.424	487.658	1193.535	-62.343
1100	1004.126	1549.595	975.694	631.292	487.617	1264.144	-60.028
1200	1030.804	1638.143	1027.246	733.077	488.244	1334.702	-58.097
1300	1053.318	1721.565	1077.477	837.314	489.348	1405.201	-56.461
1400	1072.454	1800.343	1126.324	943.628	490.790	1475.606	-55.054
1500	1088.824	1874.908	1173.766	1051.713	492.494	1545.903	-53.832
1600	1102.909	1945.640	1219.817	1161.317	494.320	1616.068	-52.758
1700	1115.097	2012.878	1264.506	1272.231	496.195	1686.090	-51.806
1800	1125.698	2076.922	1307.876	1384.283	498.037	1756.079	-50.959
1900	1134.965	2138.039	1349.972	1497.326	499.818	1825.903	-50.197
2000	1143.104	2196.466	1390.847	1611.239	501.484	1895.668	-49.509
2100	1150.283	2252.416	1430.551	1725.915	502.947	1965.337	-48.884
2200	1156.643	2306.077	1469.137	1841.268	504.210	2034.942	-48.315
2300	1162.300	2357.619	1506.653	1957.220	505.272	2104.497	-47.794
2400	1167.350	2407.195	1543.150	2073.708	506.051	2173.949	-47.314
2500	1171.875	2454.941	1578.672	2190.673	506.567	2243.513	-46.875
2600	1175.943	2500.984	1613.266	2308.067	506.777	2312.919	-46.466
2700	1179.613	2545.434	1646.972	2425.848	506.690	2382.417	-46.090
2800	1182.933	2588.395	1679.831	2543.978	506.276	2451.943	-45.741
2900	1185.945	2629.959	1711.882	2662.425	505.502	2521.428	-45.415
3000	1188.686	2670.211	1743.159	2781.158	504.424	2590.980	-45.112
3100	1191.187	2709.230	1773.696	2900.154	502.948	2660.474	-44.828
3200	1193.474	2747.085	1803.526	3019.389	501.126	2730.115	-44.564
3300	1195.571	2783.843	1832.678	3138.842	498.940	2799.869	-44.317
3400	1197.497	2819.563	1861.182	3258.497	496.353	2869.583	-44.085
3500	1199.271	2854.301	1889.062	3378.337	493.374	2939.358	-43.867
3600	1200.908	2888.109	1916.346	3498.347	490.032	3009.337	-43.663
3700	1202.421	2921.034	1943.057	3618.514	486.288	3079.426	-43.473
3800	1203.823	2953.119	1969.217	3738.827	482.113	3149.557	-43.293
3900	1205.124	2984.406	1994.848	3859.275	477.555	3219.731	-43.123
4000	1206.333	3014.933	2019.970	3979.849	472.597	3290.203	-42.965
4100	1207.459	3044.734	2044.603	4100.539	467.195	3360.712	-42.815
4200	1208.509	3073.844	2068.763	4221.338	461.384	3431.348	-42.674
4300	1209.490	3102.292	2092.469	4342.239	455.148	3502.017	-42.540
4400	1210.407	3130.108	2115.737	4463.234	448.498	3572.946	-42.415
4500	1211.266	3157.319	2138.582	4584.318	441.452	3644.096	-42.299
4600	1212.072	3183.950	2161.019	4705.486	433.945	3715.427	-42.189
4700	1212.829	3210.026	2183.062	4826.731	425.999	3786.782	-42.084
4800	1213.540	3235.567	2204.724	4948.050	417.666	3858.442	-41.988
4900	1214.210	3260.597	2226.018	5069.438	408.857	3930.111	-41.895
5000	1214.842	3285.134	2246.955	5190.891	399.688	4002.191	-41.810

3.579. Benzo[bc]naphtho[3,2,1-ef]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 128345-69-7
Point Group: C_s

Length: 15.90 Å
Width: 12.89 Å
Breadth: 3.893 Å
L/B Ratio: 1.234

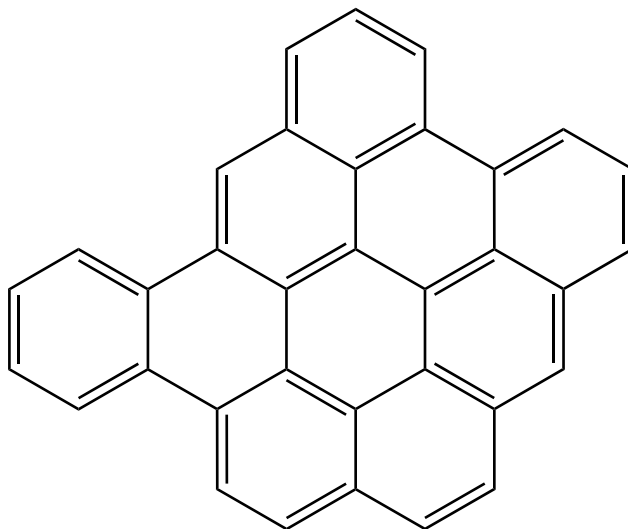
Cartesian coordinates:

C	1.0380	2.4191	0.0000	C	3.2821	1.4034	0.0000	H	2.6289	3.8583	0.0000
C	1.5388	3.7035	0.0000	C	2.1841	-1.2043	0.0000	H	1.1100	5.8248	0.0000
C	0.6751	4.8197	0.0000	C	1.3464	-0.0668	0.0000	H	-1.3568	5.5132	0.0000
C	-0.6821	4.6496	0.0000	C	-0.0549	-0.2347	0.0000	H	-3.2994	4.0284	0.0000
C	-0.9284	0.9150	0.0000	C	1.6164	-2.4878	0.0000	H	-5.9016	-2.1819	0.0000
C	-0.3772	2.2213	0.0000	C	0.2377	-2.6631	0.0000	H	-4.4094	-4.1633	0.0000
C	-1.2412	3.3411	0.0000	C	-0.6098	-1.5261	0.0000	H	-5.2579	2.5434	0.0000
C	-2.6409	3.1509	0.0000	C	-2.0323	-1.7061	0.0000	H	-6.2146	0.2558	0.0000
C	-4.8133	-2.0513	0.0000	C	-2.5844	-2.9991	0.0000	H	3.7219	2.4143	0.0000
C	-3.9835	-3.1534	0.0000	C	-1.7014	-4.1360	0.0000	H	2.2870	-3.3624	0.0000
C	-2.3166	0.7431	0.0000	C	-0.3575	-3.9759	0.0000	H	-2.1502	-5.1360	0.0000
C	-3.1801	1.8772	0.0000	C	4.1568	0.2708	0.0000	H	0.3133	-4.8428	0.0000
C	-4.6080	1.6606	0.0000	C	3.6209	-1.0289	0.0000	H	4.0713	-3.1455	0.0000
C	-5.1299	0.4137	0.0000	C	4.5009	-2.1320	0.0000	H	6.5410	-2.8024	0.0000
C	-4.2788	-0.7495	0.0000	C	5.8640	-1.9420	0.0000	H	7.4830	-0.5049	0.0000
C	-2.8850	-0.5749	0.0000	C	6.3967	-0.6422	0.0000	H	5.9676	1.4654	0.0000
C	1.9244	1.2557	0.0000	C	5.5580	0.4488	0.0000				

Table 3.579: Table of thermodynamic data as a function of temperature for Benzo[bc]naphtho[3,2,1-ef]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-57.895	504.021	504.021	∞
100	120.666	369.143	875.670	-50.653	530.806	577.710	-301.758
200	253.872	491.593	652.720	-32.225	516.597	630.295	-164.613
250	329.673	556.340	626.928	-17.647	509.944	659.488	-137.790
298.15	403.100	620.704	620.704	0.000	504.021	688.843	-120.680
300	405.883	623.206	620.712	0.748	503.801	689.987	-120.135
350	479.049	691.324	625.924	22.890	498.336	721.463	-107.670
400	546.944	759.791	638.379	48.565	493.587	753.659	-98.416
450	608.519	827.831	655.656	77.478	489.461	786.421	-91.284
500	663.599	894.851	676.235	109.308	485.863	819.639	-85.625
600	755.913	1024.337	723.556	180.469	479.939	886.980	-77.217
700	828.656	1146.542	775.344	259.839	475.523	955.197	-71.276
800	886.641	1261.120	828.984	345.709	472.456	1023.934	-66.855
900	933.552	1368.354	883.022	436.799	470.563	1092.975	-63.433
1000	972.021	1468.769	936.630	532.139	469.690	1162.186	-60.705
1100	1003.925	1562.955	989.333	630.985	469.627	1231.457	-58.476
1200	1030.634	1651.487	1040.861	732.751	470.236	1300.680	-56.616
1300	1053.174	1734.897	1091.071	836.973	471.323	1369.846	-55.040
1400	1072.331	1813.665	1139.898	943.273	472.752	1438.918	-53.686
1500	1088.717	1888.221	1187.324	1051.347	474.445	1507.883	-52.508
1600	1102.816	1958.947	1233.359	1160.941	476.261	1576.717	-51.473
1700	1115.016	2026.180	1278.034	1271.847	478.127	1645.409	-50.556
1800	1125.626	2090.219	1321.391	1383.891	479.962	1714.068	-49.740
1900	1134.901	2151.333	1363.476	1496.928	481.736	1782.562	-49.005
2000	1143.047	2209.757	1404.340	1610.834	483.396	1850.998	-48.342
2100	1150.232	2265.704	1444.035	1725.505	484.853	1919.338	-47.740
2200	1156.597	2319.363	1482.612	1840.853	486.111	1987.614	-47.191
2300	1162.258	2370.903	1520.120	1956.801	487.169	2055.841	-46.689
2400	1167.312	2420.477	1556.609	2073.284	487.945	2123.965	-46.226
2500	1171.840	2468.222	1592.124	2190.246	488.456	2192.200	-45.803
2600	1175.911	2514.263	1626.711	2307.637	488.663	2260.279	-45.409
2700	1179.583	2558.713	1660.411	2425.415	488.573	2328.448	-45.046
2800	1182.906	2601.672	1693.265	2543.542	488.156	2396.646	-44.709
2900	1185.920	2643.236	1725.310	2661.986	487.380	2464.804	-44.395
3000	1188.663	2683.487	1756.581	2780.717	486.299	2533.028	-44.103
3100	1191.165	2722.505	1787.114	2899.710	484.821	2601.195	-43.829
3200	1193.454	2760.359	1816.940	3018.943	482.997	2669.509	-43.574
3300	1195.551	2797.116	1846.088	3138.394	480.809	2737.935	-43.337
3400	1197.479	2832.836	1874.587	3258.047	478.220	2806.322	-43.113
3500	1199.254	2867.574	1902.464	3377.885	475.240	2874.770	-42.903
3600	1200.892	2901.381	1929.744	3497.894	471.896	2943.421	-42.707
3700	1202.406	2934.305	1956.452	3618.060	468.150	3012.183	-42.524
3800	1203.809	2966.390	1982.608	3738.371	463.974	3080.987	-42.350
3900	1205.111	2997.677	2008.236	3858.818	459.415	3149.834	-42.186
4000	1206.321	3028.203	2033.356	3979.390	454.455	3218.978	-42.035
4100	1207.447	3058.004	2057.985	4100.079	449.052	3288.161	-41.891
4200	1208.498	3087.114	2082.143	4220.877	443.240	3357.470	-41.755
4300	1209.479	3115.562	2105.846	4341.776	437.003	3426.811	-41.627
4400	1210.397	3143.378	2129.112	4462.771	430.351	3496.413	-41.507
4500	1211.256	3170.589	2151.954	4583.854	423.304	3566.237	-41.395
4600	1212.063	3197.220	2174.389	4705.020	415.797	3636.240	-41.290
4700	1212.820	3223.295	2196.430	4826.265	407.849	3706.269	-41.190
4800	1213.532	3248.836	2218.090	4947.583	399.515	3776.602	-41.097
4900	1214.202	3273.865	2239.382	5068.970	390.706	3846.944	-41.008
5000	1214.834	3298.402	2260.318	5190.422	381.536	3917.697	-40.927

3.580. Tribenzo[*a,ef,hi*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 128345-70-0
Point Group: C_s

Length: 15.91 Å
Width: 12.88 Å
Breadth: 3.893 Å
L/B Ratio: 1.235

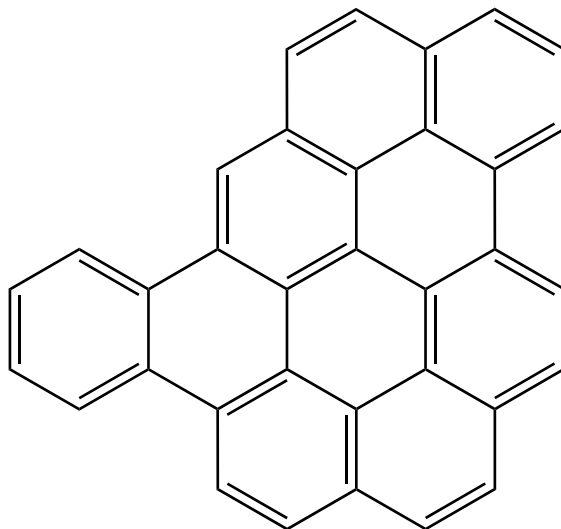
Cartesian coordinates:

C	-5.0930	1.1538	0.0000	C	-2.8687	-3.4745	0.0000	H	-5.7740	2.0124	0.0000
C	-5.5801	-0.1269	0.0000	C	-1.9700	-4.5571	0.0000	H	-6.6597	-0.3103	0.0000
C	-4.7006	-1.2273	0.0000	C	-0.6160	-4.3378	0.0000	H	-5.1033	-2.2521	0.0000
C	-3.6921	1.3875	0.0000	C	-1.0051	-1.9249	0.0000	H	-3.8743	3.5514	0.0000
C	-3.1754	2.7058	0.0000	C	-0.1079	-3.0138	0.0000	H	0.4714	5.4995	0.0000
C	-1.8138	2.9290	0.0000	C	1.2884	-2.7683	0.0000	H	-1.9769	5.1064	0.0000
C	0.0625	4.4825	0.0000	C	-0.4893	-0.5970	0.0000	H	4.3426	2.7106	0.0000
C	-1.2702	4.2684	0.0000	C	0.8901	-0.3752	0.0000	H	2.7626	4.6275	0.0000
C	0.9960	3.3815	0.0000	C	1.7904	-1.4858	0.0000	H	-3.9539	-3.6610	0.0000
C	3.2561	2.5314	0.0000	C	2.7919	1.2104	0.0000	H	-2.3667	-5.5777	0.0000
C	2.3770	3.6016	0.0000	C	1.4044	0.9676	0.0000	H	0.0878	-5.1778	0.0000
C	0.5042	2.0590	0.0000	C	3.7171	0.0850	0.0000	H	1.9824	-3.6244	0.0000
C	-0.9102	1.8229	0.0000	C	3.2275	-1.2328	0.0000	H	3.7479	-3.3304	0.0000
C	-1.4039	0.5156	0.0000	C	4.1388	-2.3012	0.0000	H	6.2013	-2.9150	0.0000
C	-2.8067	0.2859	0.0000	C	5.5026	-2.0723	0.0000	H	7.0681	-0.5814	0.0000
C	-3.3330	-1.0405	0.0000	C	5.9886	-0.7636	0.0000	H	5.4804	1.3349	0.0000
C	-2.4093	-2.1713	0.0000	C	5.1050	0.3000	0.0000				

Table 3.580: Table of thermodynamic data as a function of temperature for Tribenzo[*a,ef,hi*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-58.067	506.746	506.746	∞
100	121.571	370.727	878.183	-50.746	533.438	580.184	-303.051
200	254.318	493.705	654.929	-32.245	519.303	632.579	-165.209
250	329.847	558.520	629.126	-17.651	512.664	661.663	-138.244
298.15	403.126	622.901	622.901	0.000	506.746	690.913	-121.043
300	405.905	625.403	622.908	0.748	506.526	692.053	-120.495
350	479.015	693.519	628.121	22.889	501.061	723.419	-107.962
400	546.903	761.980	640.575	48.562	496.310	755.505	-98.657
450	608.491	830.016	657.851	77.474	492.182	788.158	-91.485
500	663.586	897.035	678.429	109.303	488.582	821.267	-85.795
600	755.912	1026.519	725.748	180.463	482.658	888.390	-77.340
700	828.642	1148.724	777.535	259.832	478.242	956.388	-71.365
800	886.602	1263.298	831.173	345.700	475.172	1024.908	-66.918
900	933.487	1370.526	885.210	436.785	473.274	1093.730	-63.477
1000	971.933	1470.934	938.816	532.117	472.393	1162.725	-60.733
1100	1003.820	1565.110	991.516	630.953	472.321	1231.780	-58.491
1200	1030.518	1653.632	1043.042	732.709	472.918	1300.788	-56.621
1300	1053.051	1737.032	1093.249	836.918	473.994	1369.740	-55.036
1400	1072.205	1815.792	1142.073	943.207	475.410	1438.599	-53.674
1500	1088.591	1890.339	1189.494	1051.267	477.091	1507.352	-52.490
1600	1102.692	1961.057	1235.526	1160.849	478.894	1575.975	-51.449
1700	1114.895	2028.282	1280.198	1271.742	480.748	1644.456	-50.527
1800	1125.510	2092.315	1323.551	1383.775	482.570	1712.905	-49.706
1900	1134.789	2153.422	1365.633	1496.800	484.333	1781.190	-48.967
2000	1142.939	2211.841	1406.493	1610.695	485.982	1849.417	-48.301
2100	1150.129	2267.783	1446.185	1725.356	487.429	1917.549	-47.695
2200	1156.499	2321.437	1484.758	1840.694	488.677	1985.617	-47.144
2300	1162.165	2372.972	1522.263	1956.632	489.726	2053.637	-46.639
2400	1167.224	2422.543	1558.748	2073.106	490.492	2121.554	-46.173
2500	1171.757	2470.285	1594.261	2190.059	490.995	2189.583	-45.748
2600	1175.832	2516.323	1628.845	2307.442	491.194	2257.456	-45.352
2700	1179.508	2560.769	1662.542	2425.213	491.096	2325.420	-44.987
2800	1182.834	2603.726	1695.393	2543.332	490.672	2393.412	-44.649
2900	1185.852	2645.287	1727.435	2661.769	489.889	2461.365	-44.333
3000	1188.598	2685.536	1758.705	2780.494	488.801	2529.384	-44.040
3100	1191.104	2724.551	1789.235	2899.481	487.316	2597.346	-43.764
3200	1193.395	2762.404	1819.058	3018.707	485.487	2665.455	-43.508
3300	1195.496	2799.159	1848.204	3138.153	483.293	2733.677	-43.270
3400	1197.426	2834.878	1876.701	3257.801	480.698	2801.860	-43.044
3500	1199.203	2869.614	1904.576	3377.634	477.713	2870.103	-42.833
3600	1200.844	2903.420	1931.854	3497.637	474.364	2938.551	-42.636
3700	1202.360	2936.343	1958.559	3617.798	470.614	3007.109	-42.452
3800	1203.765	2968.426	1984.715	3738.105	466.433	3075.709	-42.278
3900	1205.068	2999.712	2010.341	3858.548	461.869	3144.352	-42.113
4000	1206.280	3030.237	2035.458	3979.116	456.905	3213.293	-41.960
4100	1207.408	3060.037	2060.086	4099.801	451.498	3282.273	-41.816
4200	1208.460	3089.146	2084.242	4220.595	445.683	3351.379	-41.680
4300	1209.443	3117.593	2107.944	4341.491	439.442	3420.516	-41.550
4400	1210.362	3145.408	2131.208	4462.482	432.787	3489.915	-41.430
4500	1211.223	3172.618	2154.049	4583.561	425.737	3559.536	-41.317
4600	1212.031	3199.248	2176.482	4704.724	418.226	3629.337	-41.212
4700	1212.789	3225.323	2198.522	4825.966	410.275	3699.162	-41.111
4800	1213.502	3250.864	2220.180	4947.281	401.938	3769.293	-41.017
4900	1214.174	3275.892	2241.471	5068.665	393.126	3839.432	-40.928
5000	1214.807	3300.428	2262.405	5190.114	383.954	3909.982	-40.846

3.581. Benzo[g]naphtho[8,1,2-*abc*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 75449-86-4
Point Group: C_s

Length: 15.89 Å
Width: 12.88 Å
Breadth: 3.888 Å
L/B Ratio: 1.234

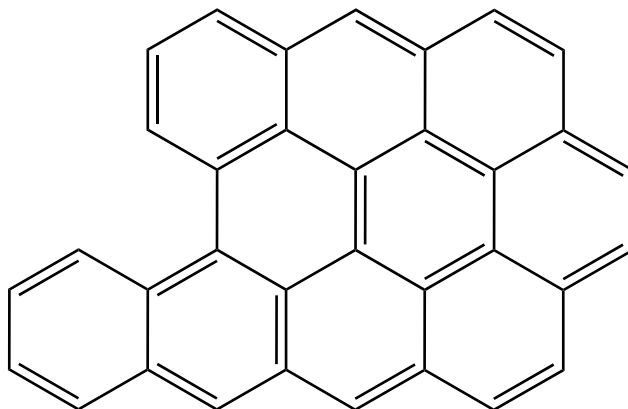
Cartesian coordinates:

C	0.4055	-2.8125	0.0000	C	-0.2779	2.2426	0.0000	H	0.8159	-3.8353	0.0000
C	-0.6206	-0.2034	0.0000	C	-3.4530	0.2102	0.0000	H	-2.5868	4.7676	0.0000
C	-2.5472	1.3459	0.0000	C	-4.8392	0.3771	0.0000	H	-4.1334	2.8150	0.0000
C	-1.1634	1.1324	0.0000	C	-5.6879	-0.7252	0.0000	H	4.9973	1.4830	0.0000
C	-2.1896	3.7461	0.0000	C	-5.1715	-2.0122	0.0000	H	4.0747	3.7914	0.0000
C	-3.0419	2.6691	0.0000	C	-2.9185	-1.0992	0.0000	H	2.1514	5.3132	0.0000
C	0.7727	-0.4130	0.0000	C	-3.7858	-2.2136	0.0000	H	-0.3059	5.6745	0.0000
C	1.2867	-1.7289	0.0000	C	-3.2258	-3.5413	0.0000	H	-5.2506	1.3983	0.0000
C	1.6707	0.7145	0.0000	C	-1.8875	-3.7350	0.0000	H	-6.7723	-0.5725	0.0000
C	3.0570	0.5234	0.0000	C	-0.9764	-2.6188	0.0000	H	-5.8449	-2.8768	0.0000
C	3.9091	1.6507	0.0000	C	-1.4984	-1.3058	0.0000	H	-3.9188	-4.3906	0.0000
C	3.4015	2.9265	0.0000	C	3.5959	-0.8253	0.0000	H	-1.4630	-4.7455	0.0000
C	1.1401	2.0330	0.0000	C	2.7270	-1.9308	0.0000	H	2.5835	-4.0891	0.0000
C	2.0057	3.1403	0.0000	C	3.2708	-3.2291	0.0000	H	5.0470	-4.4409	0.0000
C	1.4575	4.4647	0.0000	C	4.6364	-3.4260	0.0000	H	6.5841	-2.4844	0.0000
C	0.1145	4.6623	0.0000	C	5.5009	-2.3257	0.0000	H	5.6586	-0.1738	0.0000
C	-0.7911	3.5513	0.0000	C	4.9863	-1.0456	0.0000				

Table 3.581: Table of thermodynamic data as a function of temperature for Benzo[*g*]naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.920	474.639	474.639	∞
100	121.087	370.438	876.666	-50.623	501.454	548.229	-286.359
200	253.658	492.956	653.902	-32.189	487.252	600.677	-156.878
250	329.289	557.635	628.140	-17.626	480.583	629.803	-131.587
298.15	402.635	621.923	621.923	0.000	474.639	659.097	-115.469
300	405.417	624.423	621.931	0.747	474.418	660.239	-114.956
350	478.570	692.467	627.138	22.865	468.930	691.656	-103.222
400	546.490	760.871	639.580	48.517	464.157	723.797	-94.516
450	608.105	828.860	656.841	77.409	460.010	756.506	-87.811
500	663.226	895.839	677.402	109.219	456.391	789.674	-82.495
600	755.600	1025.263	724.687	180.345	450.434	856.919	-74.600
700	828.374	1147.422	776.443	259.686	445.989	925.046	-69.026
800	886.372	1261.964	830.053	345.529	442.894	993.697	-64.880
900	933.288	1369.166	884.064	436.592	440.975	1062.655	-61.674
1000	971.760	1469.554	937.648	531.906	440.075	1131.787	-59.117
1100	1003.669	1563.715	990.328	630.726	439.986	1200.980	-57.029
1200	1030.385	1652.225	1041.836	732.467	440.570	1270.129	-55.286
1300	1052.934	1735.615	1092.027	836.664	441.633	1339.222	-53.809
1400	1072.101	1814.366	1140.837	942.941	443.038	1408.223	-52.540
1500	1088.498	1888.907	1188.246	1050.992	444.709	1477.118	-51.437
1600	1102.609	1959.619	1234.266	1160.565	446.504	1545.885	-50.467
1700	1114.819	2026.839	1278.927	1271.451	448.349	1614.510	-49.607
1800	1125.441	2090.868	1322.270	1383.476	450.165	1683.103	-48.841
1900	1134.727	2151.972	1364.343	1496.494	451.921	1751.533	-48.152
2000	1142.883	2210.387	1405.196	1610.383	453.564	1819.905	-47.530
2100	1150.078	2266.327	1444.880	1725.039	455.006	1888.183	-46.965
2200	1156.452	2319.978	1483.446	1840.372	456.248	1956.397	-46.450
2300	1162.121	2371.512	1520.944	1956.306	457.293	2024.563	-45.978
2400	1167.183	2421.080	1557.424	2072.776	458.054	2092.626	-45.544
2500	1171.719	2468.821	1592.931	2189.725	458.554	2160.802	-45.147
2600	1175.797	2514.857	1627.510	2307.104	458.749	2228.820	-44.777
2700	1179.475	2559.302	1661.202	2424.871	458.648	2296.931	-44.436
2800	1182.803	2602.258	1694.048	2542.988	458.220	2365.070	-44.120
2900	1185.823	2643.818	1726.086	2661.421	457.434	2433.169	-43.825
3000	1188.571	2684.066	1757.352	2780.143	456.344	2501.335	-43.551
3100	1191.078	2723.081	1787.878	2899.128	454.856	2569.445	-43.294
3200	1193.371	2760.933	1817.698	3018.352	453.025	2637.701	-43.055
3300	1195.473	2797.687	1846.840	3137.795	450.828	2706.070	-42.833
3400	1197.405	2833.405	1875.334	3257.441	448.232	2774.400	-42.623
3500	1199.183	2868.141	1903.206	3377.271	445.244	2842.791	-42.425
3600	1200.825	2901.946	1930.481	3497.273	441.894	2911.385	-42.242
3700	1202.342	2934.868	1957.184	3617.432	438.141	2980.091	-42.070
3800	1203.748	2966.952	1983.337	3737.737	433.958	3048.838	-41.908
3900	1205.052	2998.237	2008.960	3858.178	429.393	3117.629	-41.755
4000	1206.265	3028.761	2034.075	3978.745	424.428	3186.718	-41.613
4100	1207.394	3058.561	2058.701	4099.428	419.019	3255.845	-41.479
4200	1208.446	3087.669	2082.855	4220.221	413.202	3325.099	-41.353
4300	1209.430	3116.116	2106.555	4341.115	406.960	3394.384	-41.233
4400	1210.350	3143.931	2129.816	4462.105	400.304	3463.931	-41.121
4500	1211.211	3171.141	2152.656	4583.183	393.252	3533.699	-41.017
4600	1212.019	3197.771	2175.087	4704.345	385.740	3603.647	-40.920
4700	1212.778	3223.845	2197.125	4825.586	377.788	3673.621	-40.827
4800	1213.492	3249.386	2218.782	4946.899	369.450	3743.899	-40.741
4900	1214.163	3274.414	2240.071	5068.282	360.637	3814.186	-40.659
5000	1214.796	3298.950	2261.004	5189.731	351.464	3884.884	-40.584

3.582. Benzo[bc]naphtho[1,2,3-ef]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 128345-72-2
Point Group: C₁

Length: 15.26 Å
Width: 11.77 Å
Breadth: 4.949 Å
L/B Ratio: 1.297

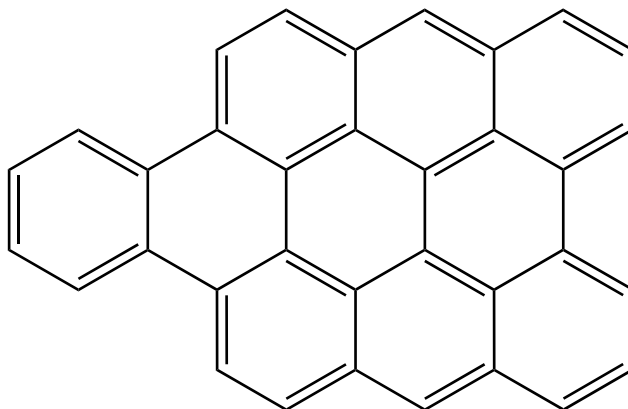
Cartesian coordinates:

C	2.9668	0.2130	0.1255	C	-2.8353	-2.6315	-0.2144	H	3.9981	-4.2818	-0.1545
C	2.5982	-1.1460	0.0045	C	-5.1963	-2.1173	0.1299	H	1.6126	-4.9246	-0.3627
C	3.5965	-2.1415	0.0009	C	-6.1786	-1.2377	0.4591	H	-0.7607	-4.2868	-0.3907
C	4.9408	-1.7732	0.1314	C	-5.8495	0.1235	0.7023	H	-3.1000	-3.6891	-0.3393
C	5.3008	-0.4404	0.2584	C	-4.5721	0.5669	0.5467	H	-5.4216	-3.1772	-0.0364
C	4.3268	0.5651	0.2528	C	1.9549	1.2244	0.1000	H	-7.2199	-1.5606	0.5575
C	1.2134	-1.4984	-0.1116	C	0.6054	0.8700	-0.0137	H	-6.6411	0.8076	1.0256
C	0.8541	-2.8816	-0.2287	C	-0.3932	1.8747	-0.1016	H	-4.3429	1.6200	0.7599
C	1.9071	-3.8743	-0.2537	C	-1.7758	1.5249	-0.2291	H	6.3573	-0.1668	0.3609
C	3.2053	-3.5250	-0.1408	C	0.0066	3.2316	-0.1256	H	5.7141	-2.5500	0.1318
C	0.2268	-0.5128	-0.1015	C	-0.9630	4.2389	-0.3647	H	-3.7175	2.3088	-0.7613
C	-1.1610	-0.8628	-0.1490	C	-2.2620	3.8841	-0.6116	H	-3.0101	4.6481	-0.8486
C	-1.4949	-2.2444	-0.2277	C	-2.6631	2.5357	-0.5520	H	-0.6528	5.2897	-0.3749
C	-0.4693	-3.2330	-0.2988	C	2.3344	2.5988	0.1647	H	1.6506	4.6373	0.0699
C	-2.1747	0.1221	-0.0791	C	1.3695	3.5770	0.0469	H	4.0044	3.9836	0.4038
C	-3.5095	-0.3039	0.1386	C	4.6784	1.9601	0.3673	H	5.7384	2.2126	0.4863
C	-3.8349	-1.6846	0.0069	C	3.7338	2.9244	0.3233				

Table 3.582: Table of thermodynamic data as a function of temperature for Benzo[bc]naphtho[1,2,3-ef]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-57.364	545.260	545.260	∞
100	117.792	358.434	863.179	-50.474	572.223	620.198	-323.952
200	253.149	479.584	640.695	-32.222	557.840	673.940	-176.011
250	329.692	544.254	614.895	-17.660	551.170	703.735	-147.034
298.15	403.597	608.666	608.666	0.000	545.260	733.671	-128.533
300	406.394	611.171	608.673	0.749	545.041	734.838	-127.944
350	479.856	679.392	613.893	22.925	539.610	766.913	-114.453
400	547.910	747.978	626.368	48.644	534.906	799.703	-104.428
450	609.553	816.136	643.674	77.608	530.830	833.053	-96.696
500	664.645	883.267	664.287	109.490	527.284	866.852	-90.558
600	756.895	1012.939	711.684	180.753	521.462	935.342	-81.427
700	829.532	1135.288	763.551	260.216	517.140	1004.691	-74.969
800	887.407	1249.976	817.265	346.168	514.154	1074.548	-70.159
900	934.219	1357.294	871.372	437.329	512.333	1144.699	-66.435
1000	972.601	1457.775	925.043	532.732	511.522	1215.013	-63.464
1100	1004.432	1552.012	977.802	631.632	511.514	1285.381	-61.036
1200	1031.079	1640.585	1029.381	733.446	512.170	1355.696	-59.011
1300	1053.567	1724.029	1079.637	837.709	513.299	1425.950	-57.294
1400	1072.680	1802.825	1128.505	944.047	514.765	1496.108	-55.819
1500	1089.028	1877.404	1175.968	1052.153	516.491	1566.156	-54.537
1600	1103.095	1948.148	1222.038	1161.777	518.337	1636.071	-53.411
1700	1115.267	2015.397	1266.744	1272.709	520.229	1705.842	-52.413
1800	1125.854	2079.450	1310.130	1384.777	522.087	1775.578	-51.525
1900	1135.108	2140.576	1352.241	1497.836	523.883	1845.148	-50.726
2000	1143.235	2199.010	1393.129	1611.761	525.563	1914.659	-50.005
2100	1150.404	2254.966	1432.846	1726.451	527.039	1984.074	-49.350
2200	1156.755	2308.632	1471.443	1841.815	528.313	2053.423	-48.753
2300	1162.404	2360.179	1508.971	1957.778	529.386	2122.723	-48.208
2400	1167.447	2409.759	1545.477	2074.275	530.175	2191.919	-47.705
2500	1171.965	2457.510	1581.010	2191.250	530.700	2261.226	-47.245
2600	1176.027	2503.556	1615.612	2308.653	530.919	2330.375	-46.817
2700	1179.692	2548.009	1649.327	2426.442	530.840	2399.615	-46.422
2800	1183.007	2590.973	1682.194	2544.580	530.434	2468.884	-46.057
2900	1186.014	2632.539	1714.252	2663.033	529.667	2538.111	-45.715
3000	1188.751	2672.794	1745.536	2781.774	528.596	2607.405	-45.398
3100	1191.248	2711.814	1776.080	2900.776	527.126	2676.641	-45.100
3200	1193.532	2749.671	1805.916	3020.016	525.310	2746.023	-44.823
3300	1195.625	2786.431	1835.074	3139.476	523.130	2815.519	-44.565
3400	1197.549	2822.153	1863.583	3259.136	520.548	2884.974	-44.321
3500	1199.320	2856.892	1891.469	3378.980	517.574	2954.490	-44.092
3600	1200.954	2890.702	1918.758	3498.995	514.237	3024.209	-43.879
3700	1202.465	2923.627	1945.474	3619.167	510.497	3094.039	-43.679
3800	1203.865	2955.714	1971.639	3739.485	506.326	3163.910	-43.490
3900	1205.164	2987.002	1997.274	3859.937	501.773	3233.825	-43.311
4000	1206.371	3017.529	2022.401	3980.514	496.818	3304.037	-43.145
4100	1207.496	3047.332	2047.037	4101.208	491.420	3374.287	-42.988
4200	1208.544	3076.442	2071.201	4222.011	485.613	3444.663	-42.840
4300	1209.523	3104.891	2094.911	4342.915	479.381	3515.072	-42.699
4400	1210.439	3132.708	2118.183	4463.913	472.733	3585.741	-42.567
4500	1211.297	3159.920	2141.031	4585.001	465.691	3656.631	-42.444
4600	1212.101	3186.552	2163.471	4706.171	458.187	3727.701	-42.329
4700	1212.857	3212.628	2185.517	4827.419	450.243	3798.797	-42.218
4800	1213.567	3238.170	2207.182	4948.741	441.913	3870.197	-42.115
4900	1214.236	3263.200	2228.479	5070.131	433.107	3941.605	-42.017
5000	1214.867	3287.737	2249.420	5191.587	423.941	4013.425	-41.927

3.583. Tribenzo[*a,hi,kl*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 128345-67-5
Point Group: C_{2v}

Length: 15.31 Å
Width: 11.68 Å
Breadth: 3.885 Å
L/B Ratio: 1.310

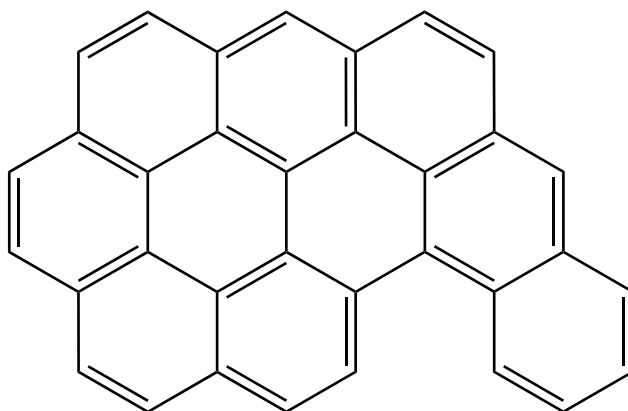
Cartesian coordinates:

C	-6.2514	0.7138	0.0000	C	-2.5548	-2.8528	0.0000	H	-7.2044	1.2528	0.0000
C	-6.2534	-0.6960	0.0000	C	-1.3866	-3.5367	0.0000	H	-7.2079	-1.2323	0.0000
C	-5.0686	-1.3844	0.0000	C	-0.1253	-2.8447	0.0000	H	-5.0574	-2.4850	0.0000
C	-5.0646	1.3988	0.0000	C	3.5670	0.7252	0.0000	H	-5.0503	2.4994	0.0000
C	-3.8238	0.7105	0.0000	C	4.7434	1.4414	0.0000	H	3.5250	-4.6468	0.0000
C	-3.8258	-0.6996	0.0000	C	4.7335	2.8542	0.0000	H	5.6794	-3.4052	0.0000
C	3.5649	-0.7354	0.0000	C	3.5521	3.5409	0.0000	H	5.7006	-0.9180	0.0000
C	3.5420	-3.5510	0.0000	C	2.3177	1.4234	0.0000	H	1.0784	-4.6340	0.0000
C	4.7253	-2.8677	0.0000	C	2.3117	2.8394	0.0000	H	-3.5208	-3.3808	0.0000
C	4.7392	-1.4549	0.0000	C	1.0871	3.5339	0.0000	H	-1.3751	-4.6327	0.0000
C	2.3136	-1.4300	0.0000	C	1.0896	0.7205	0.0000	H	5.7032	0.9018	0.0000
C	1.0876	-0.7236	0.0000	C	-0.1239	1.4213	0.0000	H	5.6891	3.3890	0.0000
C	1.0770	-3.5369	0.0000	C	-0.1171	2.8451	0.0000	H	3.5382	4.6367	0.0000
C	2.3035	-2.8460	0.0000	C	-1.3765	3.5406	0.0000	H	1.0916	4.6310	0.0000
C	-0.1279	-1.4209	0.0000	C	-2.5466	2.8601	0.0000	H	-1.3619	4.6366	0.0000
C	-1.3786	-0.7139	0.0000	C	-2.5790	1.4235	0.0000	H	-3.5112	3.3908	0.0000
C	-2.5831	-1.4162	0.0000	C	-1.3765	0.7178	0.0000				

Table 3.583: Table of thermodynamic data as a function of temperature for Tribenzo[*a,hi,kl*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.661	524.728	524.728	∞
100	119.927	357.423	863.136	-50.571	551.595	599.671	-313.229
200	253.526	479.529	640.485	-32.191	537.339	653.450	-170.660
250	329.328	544.200	614.720	-17.630	530.668	683.247	-142.754
298.15	402.743	608.501	608.501	0.000	524.728	713.188	-124.945
300	405.526	611.001	608.509	0.748	524.508	714.355	-124.378
350	478.692	679.064	613.717	22.871	519.025	746.443	-111.398
400	546.598	747.484	626.163	48.529	514.258	779.253	-101.758
450	608.189	815.484	643.427	77.425	510.115	812.631	-94.326
500	663.285	882.471	663.993	109.239	506.501	846.468	-88.428
600	755.617	1011.901	711.285	180.369	500.547	915.049	-79.660
700	828.362	1134.061	763.047	259.710	496.102	984.512	-73.464
800	886.341	1248.599	816.661	345.551	493.005	1054.500	-68.850
900	933.246	1355.798	870.675	436.610	491.082	1124.794	-65.280
1000	971.713	1456.181	924.261	531.920	490.178	1195.263	-62.433
1100	1003.619	1550.337	976.942	630.735	490.084	1265.794	-60.106
1200	1030.334	1638.842	1028.450	732.471	490.663	1336.281	-58.166
1300	1052.884	1722.228	1078.642	836.663	491.721	1406.712	-56.521
1400	1072.052	1800.976	1127.451	942.935	493.121	1477.052	-55.108
1500	1088.451	1875.513	1174.859	1050.981	494.787	1547.287	-53.880
1600	1102.564	1946.222	1220.879	1160.549	496.577	1617.393	-52.801
1700	1114.777	2013.440	1265.540	1271.431	498.419	1687.358	-51.845
1800	1125.401	2077.466	1308.882	1383.452	500.230	1757.291	-50.994
1900	1134.689	2138.568	1350.954	1496.466	501.982	1827.061	-50.228
2000	1142.847	2196.982	1391.806	1610.352	503.622	1896.774	-49.538
2100	1150.044	2252.919	1431.489	1725.004	505.060	1966.392	-48.910
2200	1156.420	2306.570	1470.054	1840.333	506.299	2035.947	-48.339
2300	1162.092	2358.102	1507.552	1956.264	507.340	2105.454	-47.815
2400	1167.155	2407.669	1544.031	2072.731	508.099	2174.858	-47.334
2500	1171.693	2455.408	1579.537	2189.678	508.596	2244.375	-46.893
2600	1175.772	2501.444	1614.115	2307.055	508.789	2313.735	-46.483
2700	1179.452	2545.888	1647.807	2424.819	508.685	2383.187	-46.105
2800	1182.781	2588.843	1680.653	2542.933	508.255	2452.667	-45.754
2900	1185.803	2630.402	1712.690	2661.365	507.467	2522.108	-45.427
3000	1188.552	2670.650	1743.955	2780.085	506.375	2591.616	-45.123
3100	1191.060	2709.664	1774.481	2899.067	504.885	2661.067	-44.838
3200	1193.354	2747.515	1804.299	3018.290	503.052	2730.664	-44.573
3300	1195.456	2784.269	1833.441	3137.732	500.854	2800.376	-44.325
3400	1197.389	2819.986	1861.935	3257.375	498.255	2870.047	-44.092
3500	1199.168	2854.721	1889.806	3377.204	495.266	2939.780	-43.873
3600	1200.810	2888.526	1917.081	3497.204	491.914	3009.717	-43.669
3700	1202.328	2921.448	1943.783	3617.362	488.160	3079.765	-43.478
3800	1203.735	2953.531	1969.935	3737.666	483.976	3149.854	-43.297
3900	1205.039	2984.816	1995.558	3858.106	479.410	3219.987	-43.126
4000	1206.253	3015.340	2020.673	3978.671	474.443	3290.418	-42.968
4100	1207.382	3045.140	2045.298	4099.354	469.033	3360.887	-42.817
4200	1208.435	3074.248	2069.451	4220.145	463.215	3431.482	-42.676
4300	1209.419	3102.694	2093.151	4341.038	456.972	3502.110	-42.541
4400	1210.339	3130.509	2116.412	4462.027	450.315	3572.999	-42.416
4500	1211.201	3157.719	2139.251	4583.104	443.262	3644.110	-42.299
4600	1212.010	3184.348	2161.682	4704.265	435.749	3715.400	-42.189
4700	1212.769	3210.422	2183.719	4825.505	427.797	3786.716	-42.084
4800	1213.483	3235.963	2205.376	4946.818	419.457	3858.337	-41.986
4900	1214.155	3260.991	2226.665	5068.200	410.644	3929.966	-41.893
5000	1214.788	3285.527	2247.597	5189.647	401.469	4002.006	-41.808

3.584. Anthra[9,1,2-*abc*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 128345-73-3
Point Group: C₁

Length: 15.53 Å
Width: 11.61 Å
Breadth: 4.916 Å
L/B Ratio: 1.337

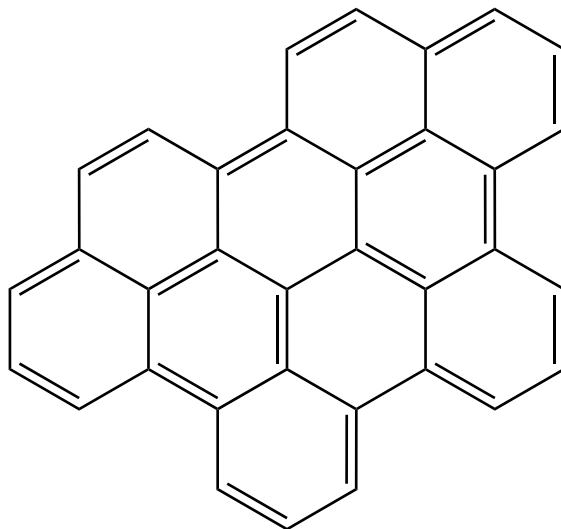
Cartesian coordinates:

C	3.6924	-3.3108	0.1134	C	2.0945	2.6399	-0.1149	H	4.5624	-3.9769	0.0908
C	2.4371	-3.8079	0.2881	C	0.9904	3.5090	-0.0022	H	2.2718	-4.8841	0.4142
C	1.3025	-2.9401	0.3068	C	0.5692	0.7274	0.0315	H	-2.0836	-3.0090	0.6693
C	1.4783	-1.5597	0.1309	C	-2.0927	-0.3126	0.0692	H	-0.1432	-4.5012	0.7317
C	-1.0855	-2.5933	0.4740	C	-4.2399	1.5370	0.2631	H	6.0640	-2.0570	-0.2173
C	-0.0069	-3.4341	0.5213	C	-0.5230	1.6000	0.1100	H	6.4154	0.3922	-0.4154
C	2.8030	-1.0394	-0.0168	C	-0.2927	3.0063	0.1216	H	5.5096	2.6812	-0.4445
C	3.9055	-1.9060	-0.0354	C	-1.4223	3.8980	0.2670	H	3.5726	4.2270	-0.3005
C	5.2118	-1.3682	-0.1907	C	-2.6762	3.4154	0.3431	H	1.1594	4.5929	-0.0092
C	5.4057	-0.0184	-0.2998	C	-2.9456	1.9953	0.2524	H	-5.0784	2.2305	0.4047
C	-0.9543	-1.2056	0.1957	C	-1.8572	1.0701	0.1480	H	-1.2230	4.9747	0.3161
C	0.3486	-0.6885	0.1076	C	-3.4478	-0.7531	-0.1397	H	-3.5342	4.0877	0.4614
C	3.0077	0.3652	-0.1272	C	-4.5090	0.1661	0.0300	H	-6.6610	0.4612	0.0987
C	4.3047	0.8784	-0.2582	C	-5.8593	-0.2621	-0.0908	H	-7.1893	-1.8828	-0.5511
C	4.4901	2.2947	-0.3325	C	-6.1517	-1.5472	-0.4560	H	-5.3400	-3.4546	-1.0878
C	3.4284	3.1414	-0.2560	C	-5.1005	-2.4450	-0.7376	H	-2.9991	-2.7729	-0.8321
C	1.8849	1.2491	-0.0751	C	-3.7957	-2.0583	-0.5846				

Table 3.584: Table of thermodynamic data as a function of temperature for Anthra[9,1,2-*abc*]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-57.194	502.477	502.477	∞
100	117.009	357.988	861.308	-50.332	529.583	577.602	-301.702
200	252.442	478.566	639.373	-32.161	515.117	631.421	-164.907
250	329.081	543.090	613.618	-17.632	508.414	661.271	-138.162
298.15	403.041	607.398	607.398	0.000	502.477	691.266	-121.104
300	405.840	609.900	607.406	0.748	502.257	692.435	-120.561
350	479.346	678.039	612.619	22.897	496.800	724.576	-108.135
400	547.439	746.560	625.080	48.592	492.071	757.435	-98.909
450	609.121	814.665	642.368	77.533	487.972	790.857	-91.798
500	664.250	881.752	662.963	109.395	484.405	824.731	-86.157
600	756.568	1011.357	710.322	180.621	478.548	893.376	-77.774
700	829.262	1133.660	762.154	260.054	474.195	962.886	-71.850
800	887.184	1248.315	815.837	345.983	471.185	1032.907	-67.441
900	934.033	1355.610	869.917	437.123	469.344	1103.225	-64.028
1000	972.446	1456.073	923.564	532.509	468.515	1173.709	-61.307
1100	1004.302	1550.297	976.302	631.395	468.493	1244.247	-59.083
1200	1030.969	1638.859	1027.862	733.197	469.137	1314.735	-57.228
1300	1053.473	1722.294	1078.102	837.450	470.256	1385.162	-55.655
1400	1072.598	1801.084	1126.956	943.779	471.713	1455.494	-54.304
1500	1088.957	1875.658	1174.406	1051.877	473.432	1525.715	-53.129
1600	1103.033	1946.398	1220.464	1161.494	475.271	1595.805	-52.097
1700	1115.212	2013.643	1265.160	1272.421	477.157	1665.751	-51.181
1800	1125.805	2077.693	1308.536	1384.484	479.010	1735.663	-50.367
1900	1135.064	2138.816	1350.639	1497.537	480.802	1805.409	-49.633
2000	1143.196	2197.249	1391.519	1611.459	482.477	1875.096	-48.971
2100	1150.369	2253.202	1431.229	1726.144	483.949	1944.687	-48.370
2200	1156.723	2306.867	1469.819	1841.505	485.220	2014.213	-47.823
2300	1162.374	2358.413	1507.341	1957.466	486.290	2083.689	-47.321
2400	1167.420	2407.991	1543.841	2073.960	487.077	2153.062	-46.859
2500	1171.940	2455.741	1579.368	2190.932	487.599	2222.546	-46.437
2600	1176.005	2501.786	1613.966	2308.333	487.815	2291.872	-46.043
2700	1179.670	2546.239	1647.676	2426.120	487.734	2361.289	-45.681
2800	1182.987	2589.202	1680.539	2544.255	487.326	2430.735	-45.345
2900	1185.996	2630.767	1712.593	2662.707	486.557	2500.139	-45.031
3000	1188.734	2671.021	1743.873	2781.445	485.484	2569.610	-44.740
3100	1191.232	2710.041	1774.413	2900.446	484.012	2639.023	-44.466
3200	1193.517	2747.898	1804.246	3019.685	482.195	2708.583	-44.212
3300	1195.611	2784.657	1833.401	3139.143	480.013	2778.256	-43.975
3400	1197.536	2820.378	1861.907	3258.801	477.430	2847.888	-43.752
3500	1199.308	2855.118	1889.791	3378.645	474.455	2917.582	-43.542
3600	1200.943	2888.927	1917.077	3498.658	471.117	2987.479	-43.346
3700	1202.454	2921.852	1943.790	3618.829	467.376	3057.486	-43.163
3800	1203.855	2953.938	1969.953	3739.146	463.204	3127.535	-42.990
3900	1205.154	2985.226	1995.586	3859.597	458.649	3197.627	-42.827
4000	1206.362	3015.753	2020.710	3980.173	453.694	3268.017	-42.675
4100	1207.487	3045.556	2045.344	4100.866	448.295	3338.444	-42.531
4200	1208.535	3074.666	2069.507	4221.668	442.487	3408.998	-42.396
4300	1209.515	3103.115	2093.214	4342.571	436.254	3479.584	-42.268
4400	1210.431	3130.932	2116.484	4463.569	429.606	3550.431	-42.148
4500	1211.289	3158.143	2139.331	4584.655	422.562	3621.499	-42.036
4600	1212.094	3184.775	2161.769	4705.825	415.058	3692.747	-41.932
4700	1212.850	3210.851	2183.814	4827.073	407.113	3764.020	-41.832
4800	1213.561	3236.393	2205.477	4948.394	398.782	3835.598	-41.739
4900	1214.230	3261.422	2226.773	5069.783	389.976	3907.184	-41.650
5000	1214.861	3285.960	2247.712	5191.238	380.809	3979.181	-41.569

3.585. Dibenzo[*fg,ij*]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 187-94-0
Point Group: C_{2v}

Length: 15.88 Å
Width: 11.66 Å
Breadth: 3.885 Å
L/B Ratio: 1.362

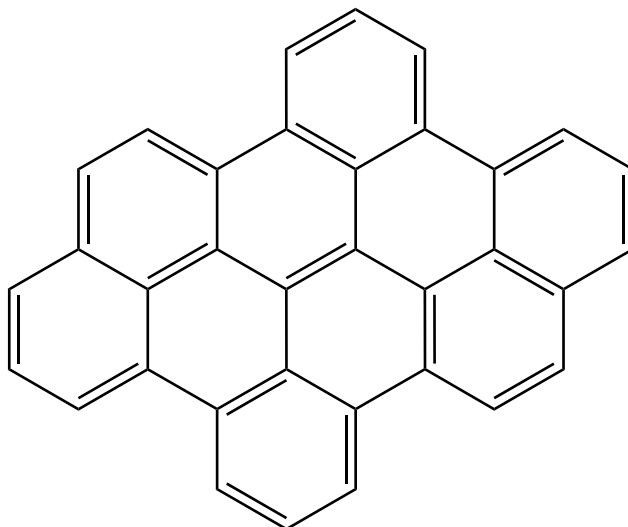
Cartesian coordinates:

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C	0.6980	0.2185	0.0000	C	-2.8444	-1.0144	0.0000	H	3.3798	4.8349	0.0000
C	1.4257	1.4638	0.0000	C	-3.5458	-2.2373	0.0000	H	0.8907	4.8430	0.0000
C	2.8399	1.4683	0.0000	C	-2.8099	-3.4674	0.0000	H	-0.8919	4.8428	0.0000
C	3.5236	2.6834	0.0000	C	-1.4545	-3.4619	0.0000	H	-3.3810	4.8341	0.0000
C	2.8286	3.8889	0.0000	C	-0.7128	-2.2341	0.0000	H	-4.6252	2.6768	0.0000
C	1.4450	3.8920	0.0000	C	-1.4084	-1.0165	0.0000	H	-5.5167	1.1192	0.0000
C	0.7262	2.6875	0.0000	C	3.5681	0.2054	0.0000	H	-6.7410	-1.0441	0.0000
C	-2.8403	1.4677	0.0000	C	4.9538	-2.2374	0.0000	H	-5.4903	-3.1939	0.0000
C	-1.4260	1.4634	0.0000	C	5.6462	-1.0442	0.0000	H	-3.3698	-4.4096	0.0000
C	-0.7268	2.6874	0.0000	C	4.9575	0.1721	0.0000	H	-0.8855	-4.4041	0.0000
C	-1.4459	3.8917	0.0000	C	3.5464	-2.2364	0.0000	H	5.4911	-3.1926	0.0000
C	-2.8295	3.8882	0.0000	C	2.8447	-1.0137	0.0000	H	6.7412	-1.0424	0.0000
C	-3.5243	2.6826	0.0000	C	1.4086	-1.0162	0.0000	H	5.5164	1.1206	0.0000
C	-3.5682	0.2045	0.0000	C	0.7134	-2.2339	0.0000	H	0.8865	-4.4039	0.0000
C	-4.9575	0.1709	0.0000	C	1.4553	-3.4615	0.0000	H	3.3708	-4.4088	0.0000
C	-5.6459	-1.0456	0.0000	C	2.8107	-3.4667	0.0000				

Table 3.585: Table of thermodynamic data as a function of temperature for Dibenzofg,ijphenanthro[2,1,10,9,8,7-pqrstuv]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-57.714	496.212	496.212	∞
100	120.527	362.104	867.031	-50.493	523.157	570.765	-298.131
200	253.002	484.265	644.822	-32.111	508.903	624.066	-162.986
250	328.478	548.779	619.121	-17.585	502.197	653.631	-136.566
298.15	401.767	612.918	612.918	0.000	496.212	683.355	-119.719
300	404.548	615.412	612.926	0.746	495.990	684.514	-119.182
350	477.721	683.323	618.122	22.820	490.458	716.385	-106.912
400	545.700	751.618	630.541	48.431	485.645	748.986	-97.805
450	607.386	819.518	647.773	77.285	481.459	782.160	-90.789
500	662.574	886.425	668.303	109.061	477.807	815.796	-85.224
600	755.052	1015.739	715.526	180.128	471.790	883.989	-76.957
700	827.889	1137.819	767.224	259.417	467.293	953.072	-71.118
800	885.924	1252.299	820.782	345.213	464.151	1022.687	-66.773
900	932.864	1359.450	874.747	436.233	462.189	1092.614	-63.412
1000	971.357	1459.794	928.288	531.506	461.247	1162.720	-60.733
1100	1003.284	1553.918	980.930	630.286	461.120	1232.891	-58.544
1200	1030.020	1642.395	1032.403	731.990	461.666	1303.021	-56.718
1300	1052.588	1725.756	1082.563	836.151	462.693	1373.099	-55.171
1400	1071.774	1804.482	1131.343	942.395	464.065	1443.087	-53.841
1500	1088.190	1879.001	1178.725	1050.414	465.704	1512.972	-52.685
1600	1102.320	1949.694	1224.721	1159.957	467.469	1582.730	-51.670
1700	1114.548	2016.897	1269.359	1270.814	469.286	1652.349	-50.769
1800	1125.187	2080.911	1312.681	1382.813	471.075	1721.937	-49.968
1900	1134.489	2142.001	1354.734	1495.807	472.807	1791.363	-49.247
2000	1142.660	2200.405	1395.569	1609.673	474.427	1860.733	-48.596
2100	1149.869	2256.334	1435.235	1724.307	475.847	1930.009	-48.005
2200	1156.256	2309.976	1473.785	1839.620	477.070	1999.223	-47.467
2300	1161.937	2361.502	1511.269	1955.535	478.095	2068.390	-46.974
2400	1167.010	2411.062	1547.734	2071.987	478.839	2137.454	-46.520
2500	1171.556	2458.796	1583.228	2188.919	479.321	2206.632	-46.104
2600	1175.644	2504.826	1617.794	2306.283	479.501	2275.653	-45.717
2700	1179.331	2549.266	1651.475	2424.035	479.385	2344.767	-45.361
2800	1182.668	2592.217	1684.310	2542.138	478.944	2413.910	-45.031
2900	1185.695	2633.772	1716.338	2660.558	478.144	2483.014	-44.723
3000	1188.450	2674.016	1747.593	2779.268	477.042	2552.185	-44.437
3100	1190.963	2713.026	1778.110	2898.240	475.542	2621.299	-44.168
3200	1193.262	2750.875	1807.921	3017.453	473.699	2690.561	-43.918
3300	1195.370	2787.626	1837.054	3136.886	471.492	2759.937	-43.685
3400	1197.307	2823.341	1865.540	3256.521	468.885	2829.272	-43.466
3500	1199.090	2858.074	1893.404	3376.342	465.888	2898.670	-43.259
3600	1200.736	2891.876	1920.672	3496.335	462.529	2968.272	-43.068
3700	1202.257	2924.796	1947.368	3616.485	458.767	3037.985	-42.888
3800	1203.667	2956.877	1973.514	3736.783	454.576	3107.739	-42.718
3900	1204.975	2988.160	1999.131	3857.215	450.003	3177.537	-42.557
4000	1206.191	3018.683	2024.240	3977.774	445.030	3247.634	-42.409
4100	1207.323	3048.481	2048.859	4098.451	439.615	3317.769	-42.268
4200	1208.379	3077.588	2073.007	4219.237	433.790	3388.030	-42.135
4300	1209.365	3106.033	2096.702	4340.124	427.542	3458.324	-42.009
4400	1210.288	3133.846	2119.958	4461.107	420.879	3528.879	-41.892
4500	1211.152	3161.055	2142.793	4582.180	413.822	3599.656	-41.783
4600	1211.962	3187.684	2165.219	4703.336	406.304	3670.613	-41.680
4700	1212.723	3213.757	2187.252	4824.571	398.347	3741.595	-41.582
4800	1213.439	3239.296	2208.905	4945.879	390.003	3812.883	-41.492
4900	1214.113	3264.323	2230.189	5067.257	381.185	3884.179	-41.405
5000	1214.748	3288.858	2251.118	5188.700	372.006	3955.886	-41.326

3.586. Perylo[3,2,1,12-*pqrab*]perylene



Formula: $C_{34}H_{16}$
Mass: 424.491 g/mol
CAS Number: 187-95-1
Point Group: C_{2h}

Length: 15.89 Å
Width: 11.65 Å
Breadth: 3.889 Å
L/B Ratio: 1.364

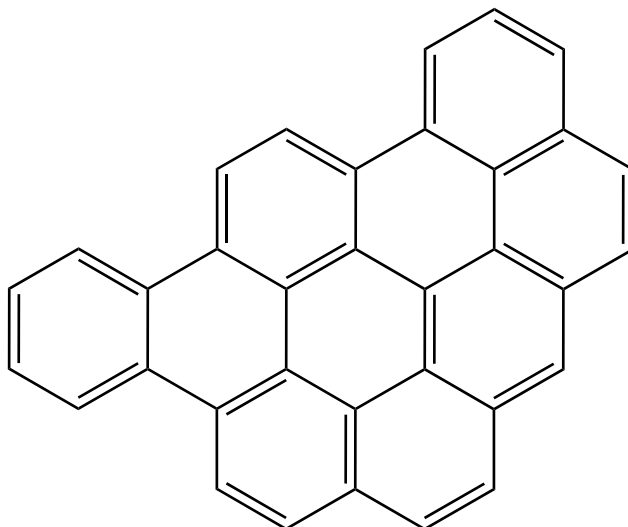
Cartesian coordinates:

C	-0.0832	-2.5641	0.0000	C	-4.8118	-1.1881	0.0000	H	-3.8620	-3.5315	0.0000
C	-2.7957	-3.2574	0.0000	C	-1.6785	0.8535	0.0000	H	-2.1192	-5.3086	0.0000
C	-1.8167	-4.2563	0.0000	C	-1.3118	2.1989	0.0000	H	0.2935	-4.6973	0.0000
C	-0.4826	-3.9169	0.0000	C	-2.3293	3.2019	0.0000	H	3.8620	3.5315	0.0000
C	2.4404	1.9161	0.0000	C	-3.6472	2.8691	0.0000	H	2.1194	5.3085	0.0000
C	2.7958	3.2573	0.0000	C	-4.0496	1.4982	0.0000	H	-0.2935	4.6973	0.0000
C	1.8168	4.2562	0.0000	C	-3.0645	0.4902	0.0000	H	-6.1744	1.9363	0.0000
C	0.4826	3.9169	0.0000	C	3.4619	0.8737	0.0000	H	-6.8454	-0.4592	0.0000
C	0.6740	0.1733	0.0000	C	5.4166	-1.1446	0.0000	H	-5.1176	-2.2458	0.0000
C	1.0668	1.5539	0.0000	C	5.7864	0.1804	0.0000	H	-2.0140	4.2566	0.0000
C	0.0832	2.5641	0.0000	C	4.8118	1.1882	0.0000	H	-4.4230	3.6434	0.0000
C	-1.0668	-1.5540	0.0000	C	4.0496	-1.4982	0.0000	H	6.1743	-1.9363	0.0000
C	-0.6740	-0.1733	0.0000	C	3.0644	-0.4902	0.0000	H	6.8453	0.4594	0.0000
C	-2.4404	-1.9161	0.0000	C	1.6784	-0.8535	0.0000	H	5.1175	2.2458	0.0000
C	-3.4619	-0.8737	0.0000	C	1.3118	-2.1990	0.0000	H	2.0141	-4.2566	0.0000
C	-5.4166	1.1447	0.0000	C	2.3294	-3.2019	0.0000	H	4.4230	-3.6433	0.0000
C	-5.7864	-0.1804	0.0000	C	3.6473	-2.8690	0.0000				

Table 3.586: Table of thermodynamic data as a function of temperature for Perylo[3,2,1,12-*pqrab*]perylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-57.725	500.838	500.838	∞
100	120.708	363.606	868.168	-50.456	527.820	575.277	-300.488
200	252.756	485.712	646.139	-32.085	513.554	628.429	-164.125
250	328.209	550.169	620.458	-17.572	506.836	657.922	-137.463
298.15	401.489	614.260	614.260	0.000	500.838	687.581	-120.459
300	404.270	616.752	614.267	0.745	500.615	688.737	-119.917
350	477.430	684.619	619.460	22.806	495.069	720.542	-107.533
400	545.397	752.874	631.871	48.401	490.241	753.079	-98.340
450	607.074	820.738	649.093	77.240	486.040	786.192	-91.257
500	662.260	887.611	669.611	109.000	482.372	819.768	-85.639
600	754.745	1016.869	716.809	180.036	476.324	887.845	-77.292
700	827.598	1138.903	768.482	259.295	471.797	956.818	-71.397
800	885.653	1253.345	822.015	345.064	468.627	1026.326	-67.011
900	932.614	1360.465	875.958	436.057	466.639	1096.150	-63.618
1000	971.126	1460.784	929.479	531.306	465.673	1166.155	-60.912
1100	1003.073	1554.887	982.101	630.064	465.524	1236.229	-58.702
1200	1029.825	1643.346	1033.557	731.747	466.049	1306.263	-56.859
1300	1052.409	1726.693	1083.700	835.890	467.058	1376.246	-55.297
1400	1071.610	1805.406	1132.466	942.117	468.412	1446.141	-53.955
1500	1088.039	1879.914	1179.834	1050.120	470.036	1515.934	-52.788
1600	1102.181	1950.597	1225.817	1159.648	471.786	1585.602	-51.764
1700	1114.420	2017.793	1270.444	1270.493	473.590	1655.130	-50.855
1800	1125.069	2081.799	1313.755	1382.479	475.367	1724.629	-50.046
1900	1134.380	2142.884	1355.799	1495.462	477.088	1793.967	-49.319
2000	1142.559	2201.282	1396.623	1609.318	478.697	1863.249	-48.662
2100	1149.775	2257.206	1436.282	1723.942	480.107	1932.438	-48.066
2200	1156.169	2310.844	1474.824	1839.245	481.321	2001.565	-47.522
2300	1161.856	2362.366	1512.300	1955.152	482.338	2070.644	-47.025
2400	1166.935	2411.923	1548.758	2071.596	483.074	2139.623	-46.567
2500	1171.486	2459.654	1584.245	2188.521	483.549	2208.714	-46.148
2600	1175.578	2505.681	1618.805	2305.878	483.722	2277.650	-45.758
2700	1179.269	2550.119	1652.480	2423.623	483.599	2346.679	-45.398
2800	1182.609	2593.067	1685.310	2541.720	483.152	2415.737	-45.065
2900	1185.640	2634.620	1717.332	2660.135	482.347	2484.756	-44.754
3000	1188.398	2674.862	1748.583	2778.839	481.239	2553.842	-44.465
3100	1190.914	2713.871	1779.095	2897.806	479.734	2622.872	-44.194
3200	1193.216	2751.718	1808.901	3017.015	477.886	2692.049	-43.942
3300	1195.326	2788.468	1838.031	3136.443	475.675	2761.340	-43.707
3400	1197.265	2824.181	1866.513	3256.074	473.064	2830.592	-43.486
3500	1199.051	2858.913	1894.373	3375.891	470.063	2899.905	-43.278
3600	1200.698	2892.715	1921.637	3495.880	466.700	2969.423	-43.084
3700	1202.222	2925.634	1948.329	3616.027	462.934	3039.052	-42.903
3800	1203.633	2957.714	1974.472	3736.320	458.740	3108.723	-42.731
3900	1204.943	2988.996	2000.086	3856.750	454.164	3178.438	-42.570
4000	1206.160	3019.518	2025.192	3977.306	449.188	3248.450	-42.420
4100	1207.294	3049.316	2049.809	4097.979	443.769	3318.502	-42.277
4200	1208.351	3078.421	2073.954	4218.762	437.942	3388.680	-42.144
4300	1209.338	3106.866	2097.646	4339.647	431.691	3458.890	-42.016
4400	1210.262	3134.679	2120.900	4460.628	425.025	3529.362	-41.898
4500	1211.127	3161.887	2143.732	4581.697	417.965	3600.056	-41.788
4600	1211.938	3188.515	2166.156	4702.851	410.445	3670.930	-41.684
4700	1212.700	3214.587	2188.187	4824.083	402.485	3741.829	-41.585
4800	1213.417	3240.126	2209.837	4945.390	394.139	3813.033	-41.493
4900	1214.092	3265.153	2231.119	5066.765	385.319	3884.246	-41.406
5000	1214.727	3289.688	2252.046	5188.207	376.138	3955.870	-41.326

3.587. Benzo[*m*]naphtho[8,1,2-*abc*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 75449-99-9
Point Group: C_s

Length: 15.93 Å
Width: 11.64 Å
Breadth: 3.886 Å
L/B Ratio: 1.368

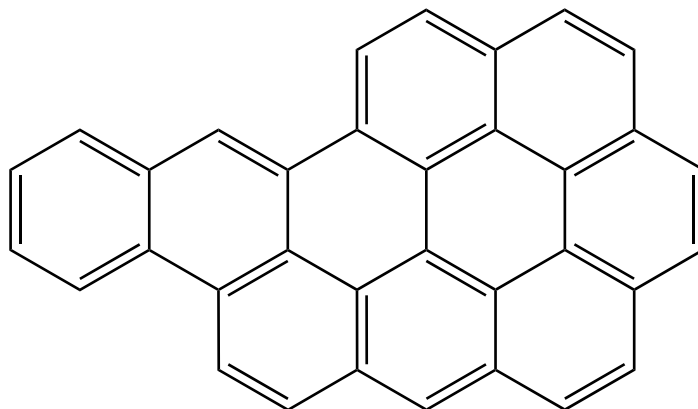
Cartesian coordinates:

C	1.2139	-2.9751	0.0000	C	-0.6872	4.2586	0.0000	H	1.8389	-3.8814	0.0000
C	-0.1586	-3.0746	0.0000	C	-2.4157	-2.0243	0.0000	H	-0.6508	-4.0596	0.0000
C	-0.9661	-1.9217	0.0000	C	-5.2207	-2.1855	0.0000	H	-3.3446	3.7807	0.0000
C	-0.3529	-0.6590	0.0000	C	-4.4504	-3.3396	0.0000	H	4.7707	2.2165	0.0000
C	1.0624	-0.5556	0.0000	C	-3.0620	-3.2627	0.0000	H	3.3670	4.2690	0.0000
C	1.8492	-1.7183	0.0000	C	-3.1940	-0.8444	0.0000	H	1.1582	5.3353	0.0000
C	-1.1575	0.5372	0.0000	C	-2.5600	0.4435	0.0000	H	-1.3170	5.1558	0.0000
C	-2.7327	2.8702	0.0000	C	-3.3486	1.6210	0.0000	H	-6.3145	-2.2526	0.0000
C	1.6904	0.7417	0.0000	C	-4.7857	1.4970	0.0000	H	-4.9379	-4.3203	0.0000
C	3.0865	0.8578	0.0000	C	-5.3819	0.2842	0.0000	H	-2.4521	-4.1792	0.0000
C	3.6722	2.1432	0.0000	C	-4.6036	-0.9296	0.0000	H	-5.3800	2.4181	0.0000
C	2.8982	3.2784	0.0000	C	3.9053	-0.3400	0.0000	H	-6.4742	0.1925	0.0000
C	-1.3361	2.9757	0.0000	C	3.2962	-1.6073	0.0000	H	3.6213	-3.7461	0.0000
C	-0.5429	1.8066	0.0000	C	4.1080	-2.7587	0.0000	H	6.1038	-3.5567	0.0000
C	0.8878	1.9137	0.0000	C	5.4828	-2.6551	0.0000	H	7.1815	-1.3144	0.0000
C	1.4906	3.1820	0.0000	C	6.0895	-1.3928	0.0000	H	5.7784	0.7423	0.0000
C	0.6644	4.3567	0.0000	C	5.3115	-0.2546	0.0000				

Table 3.587: Table of thermodynamic data as a function of temperature for Benzo[*m*]naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.522	475.091	475.091	∞
100	119.725	365.666	869.274	-50.361	502.169	549.420	-286.982
200	252.346	487.236	647.554	-32.064	487.830	602.399	-157.327
250	328.012	551.627	621.887	-17.565	481.096	631.819	-132.009
298.15	401.375	615.692	615.692	0.000	475.091	661.408	-115.874
300	404.157	618.183	615.699	0.745	474.869	662.561	-115.360
350	477.330	686.035	620.891	22.800	469.318	694.295	-103.616
400	545.282	754.275	633.299	48.390	464.484	726.762	-94.903
450	606.941	822.124	650.517	77.223	460.277	759.805	-88.194
500	662.117	888.983	671.031	108.976	456.602	793.312	-82.875
600	754.615	1018.215	718.218	179.998	450.539	861.253	-74.977
700	827.512	1140.232	769.881	259.246	446.002	930.092	-69.403
800	885.620	1254.666	823.405	345.009	442.826	999.468	-65.257
900	932.631	1361.786	877.340	436.001	440.837	1069.160	-62.051
1000	971.185	1462.109	930.855	531.254	439.875	1139.033	-59.496
1100	1003.162	1556.218	983.473	630.020	439.733	1208.974	-57.408
1200	1029.937	1644.686	1034.925	731.713	440.269	1278.874	-55.667
1300	1052.535	1728.043	1085.067	835.868	441.290	1348.723	-54.191
1400	1071.744	1806.766	1133.832	942.108	442.657	1418.483	-52.923
1500	1088.177	1881.283	1181.200	1050.125	444.294	1488.139	-51.821
1600	1102.319	1951.975	1227.183	1159.667	446.058	1557.669	-50.852
1700	1114.557	2019.179	1271.811	1270.525	447.876	1627.060	-49.992
1800	1125.202	2083.193	1315.124	1382.525	449.666	1696.420	-49.228
1900	1134.509	2144.285	1357.169	1495.521	451.400	1765.617	-48.539
2000	1142.683	2202.690	1397.995	1609.389	453.023	1834.759	-47.918
2100	1149.894	2258.620	1437.655	1724.025	454.445	1903.807	-47.354
2200	1156.282	2312.263	1476.199	1839.340	455.670	1972.792	-46.839
2300	1161.965	2363.790	1513.677	1955.258	456.698	2041.730	-46.368
2400	1167.038	2413.352	1550.138	2071.713	457.445	2110.566	-45.934
2500	1171.584	2461.086	1585.627	2188.648	457.930	2179.514	-45.538
2600	1175.671	2507.118	1620.189	2306.015	458.112	2248.307	-45.168
2700	1179.358	2551.558	1653.866	2423.769	457.999	2317.191	-44.828
2800	1182.694	2594.510	1686.698	2541.875	457.560	2386.105	-44.512
2900	1185.721	2636.066	1718.722	2660.298	456.763	2454.980	-44.218
3000	1188.475	2676.311	1749.974	2779.010	455.663	2523.921	-43.944
3100	1190.988	2715.322	1780.488	2897.985	454.166	2592.806	-43.688
3200	1193.286	2753.171	1810.296	3017.200	452.325	2661.838	-43.449
3300	1195.393	2789.923	1839.428	3136.635	450.121	2730.984	-43.227
3400	1197.329	2825.639	1867.911	3256.273	447.516	2800.090	-43.017
3500	1199.111	2860.372	1895.773	3376.096	444.521	2869.257	-42.820
3600	1200.756	2894.176	1923.039	3496.091	441.164	2938.629	-42.638
3700	1202.277	2927.096	1949.733	3616.243	437.405	3008.112	-42.466
3800	1203.686	2959.178	1975.877	3736.542	433.216	3077.637	-42.304
3900	1204.993	2990.461	2001.493	3856.977	428.644	3147.205	-42.151
4000	1206.209	3020.984	2026.600	3977.538	423.673	3217.071	-42.010
4100	1207.340	3050.783	2051.218	4098.216	418.259	3286.976	-41.876
4200	1208.395	3079.890	2075.365	4219.003	412.437	3357.007	-41.750
4300	1209.381	3108.336	2099.058	4339.893	406.190	3427.071	-41.630
4400	1210.303	3136.149	2122.314	4460.877	399.529	3497.396	-41.519
4500	1211.166	3163.358	2145.147	4581.951	392.473	3567.942	-41.415
4600	1211.976	3189.987	2167.572	4703.109	384.956	3638.669	-41.318
4700	1212.737	3216.060	2189.604	4824.345	377.000	3709.421	-41.225
4800	1213.452	3241.600	2211.255	4945.655	368.658	3780.478	-41.139
4900	1214.125	3266.628	2232.539	5067.034	359.841	3851.544	-41.057
5000	1214.760	3291.163	2253.467	5188.479	350.664	3923.020	-40.983

3.588. Phenanthro[10,1,2-*abc*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 75459-01-7
Point Group: C_s

Length: 16.55 Å
Width: 11.66 Å
Breadth: 3.886 Å
L/B Ratio: 1.420

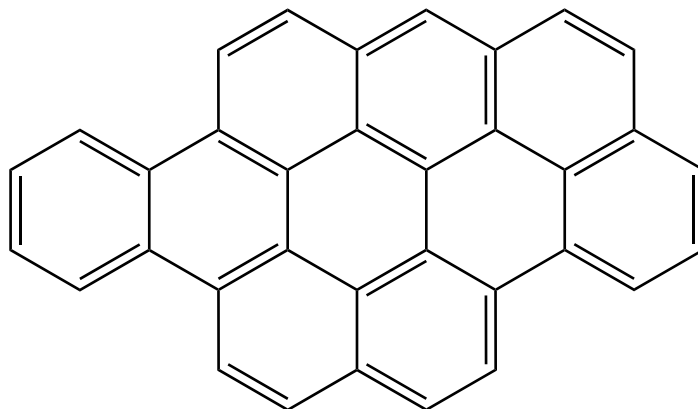
Cartesian coordinates:

C	-0.4520	-3.3696	0.0000	C	-2.0238	2.9204	0.0000	H	-0.3942	-4.4651	0.0000
C	-0.5929	-0.5591	0.0000	C	-3.3154	3.5415	0.0000	H	1.3175	3.6579	0.0000
C	-0.6648	0.8824	0.0000	C	-4.4503	2.7945	0.0000	H	-0.9046	4.7779	0.0000
C	0.5000	1.6561	0.0000	C	1.8037	1.0054	0.0000	H	-5.0581	-3.4666	0.0000
C	0.3902	3.0640	0.0000	C	2.9696	1.7370	0.0000	H	-2.8485	-4.5941	0.0000
C	-0.8367	3.6840	0.0000	C	3.1089	-1.0753	0.0000	H	-6.5378	1.0714	0.0000
C	-1.6992	-2.7419	0.0000	C	1.8701	-0.4258	0.0000	H	-6.3969	-1.4061	0.0000
C	-1.7718	-1.3278	0.0000	C	0.6614	-1.1995	0.0000	H	-3.3636	4.6365	0.0000
C	-4.1293	-2.8846	0.0000	C	0.7244	-2.6147	0.0000	H	-5.4371	3.2714	0.0000
C	-2.9217	-3.5004	0.0000	C	2.0128	-3.2490	0.0000	H	2.9196	2.8381	0.0000
C	-4.2284	-1.4517	0.0000	C	3.1486	-2.5103	0.0000	H	2.0529	-4.3443	0.0000
C	-3.0553	-0.6862	0.0000	C	4.2362	1.1005	0.0000	H	4.1399	-2.9895	0.0000
C	-5.5625	0.5713	0.0000	C	4.3160	-0.3071	0.0000	H	5.6460	-2.0201	0.0000
C	-5.4845	-0.7986	0.0000	C	5.5970	-0.9205	0.0000	H	7.7215	-0.6383	0.0000
C	-4.3882	1.3631	0.0000	C	6.7360	-0.1612	0.0000	H	7.5761	1.8384	0.0000
C	-3.1343	0.7332	0.0000	C	6.6531	1.2495	0.0000	H	5.3585	2.9620	0.0000
C	-1.9355	1.5168	0.0000	C	5.4322	1.8685	0.0000				

Table 3.588: Table of thermodynamic data as a function of temperature for Phenanthro[10,1,2-*abc*]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-57.447	478.525	478.525	∞
100	118.839	363.688	867.501	-50.381	505.582	553.031	-288.868
200	252.523	484.943	645.559	-32.123	491.203	606.232	-158.328
250	328.658	549.427	619.841	-17.604	484.491	635.764	-132.833
298.15	402.296	613.631	613.631	0.000	478.525	665.456	-116.583
300	405.085	616.128	613.639	0.747	478.304	666.613	-116.065
350	478.386	684.134	618.842	22.852	472.803	698.446	-104.235
400	546.367	752.518	631.278	48.496	468.023	731.004	-95.457
450	608.003	820.494	648.533	77.383	463.869	764.131	-88.696
500	663.130	887.463	669.088	109.188	460.246	797.717	-83.335
600	755.518	1016.870	716.361	180.305	454.280	865.801	-75.373
700	828.318	1139.019	768.106	259.639	449.827	934.767	-69.752
800	886.349	1253.555	821.707	345.478	446.729	1004.259	-65.570
900	933.298	1360.756	875.712	436.540	444.809	1074.058	-62.335
1000	971.799	1461.147	929.290	531.857	443.912	1144.031	-59.757
1100	1003.730	1555.313	981.966	630.682	443.828	1214.065	-57.650
1200	1030.461	1643.828	1033.470	732.430	444.419	1284.053	-55.892
1300	1053.020	1727.225	1083.660	836.635	445.490	1353.986	-54.403
1400	1072.193	1805.983	1132.468	942.921	446.904	1423.826	-53.122
1500	1088.593	1880.530	1179.876	1050.981	448.584	1493.559	-52.009
1600	1102.704	1951.248	1225.896	1160.564	450.388	1563.163	-51.031
1700	1114.914	2018.474	1270.557	1271.459	452.244	1632.625	-50.163
1800	1125.534	2082.508	1313.901	1383.493	454.068	1702.054	-49.391
1900	1134.817	2143.617	1355.974	1496.521	455.834	1771.320	-48.696
2000	1142.969	2202.037	1396.828	1610.419	457.486	1840.527	-48.069
2100	1150.161	2257.981	1436.512	1725.083	458.936	1909.640	-47.499
2200	1156.531	2311.636	1475.080	1840.424	460.187	1978.688	-46.979
2300	1162.197	2363.173	1512.579	1956.366	461.239	2047.688	-46.504
2400	1167.256	2412.745	1549.060	2072.843	462.008	2116.585	-46.065
2500	1171.788	2460.488	1584.568	2189.799	462.514	2185.594	-45.665
2600	1175.863	2506.527	1619.148	2307.185	462.716	2254.446	-45.291
2700	1179.538	2550.975	1652.842	2424.959	462.621	2323.389	-44.948
2800	1182.863	2593.933	1685.690	2543.081	462.200	2392.361	-44.629
2900	1185.880	2635.495	1717.729	2661.521	461.420	2461.293	-44.332
3000	1188.625	2675.745	1748.995	2780.248	460.335	2530.291	-44.055
3100	1191.130	2714.761	1779.523	2899.238	458.853	2599.232	-43.796
3200	1193.420	2752.614	1809.344	3018.467	457.026	2668.320	-43.555
3300	1195.520	2789.371	1838.487	3137.916	454.834	2737.522	-43.330
3400	1197.449	2825.089	1866.982	3257.565	452.242	2806.683	-43.119
3500	1199.226	2859.827	1894.855	3377.400	449.259	2875.905	-42.920
3600	1200.865	2893.633	1922.131	3497.406	445.913	2945.331	-42.735
3700	1202.381	2926.556	1948.835	3617.569	442.164	3014.868	-42.561
3800	1203.785	2958.641	1974.989	3737.878	437.985	3084.447	-42.398
3900	1205.088	2989.927	2000.613	3858.323	433.424	3154.069	-42.243
4000	1206.299	3020.452	2025.729	3978.893	428.462	3223.988	-42.100
4100	1207.426	3050.253	2050.356	4099.580	423.057	3293.946	-41.965
4200	1208.478	3079.362	2074.510	4220.376	417.242	3364.030	-41.837
4300	1209.460	3107.810	2098.211	4341.273	411.004	3434.147	-41.716
4400	1210.378	3135.625	2121.474	4462.265	404.350	3504.524	-41.603
4500	1211.239	3162.835	2144.314	4583.347	397.302	3575.123	-41.498
4600	1212.046	3189.466	2166.746	4704.511	389.792	3645.902	-41.400
4700	1212.804	3215.541	2188.785	4825.754	381.843	3716.706	-41.306
4800	1213.516	3241.082	2210.442	4947.071	373.508	3787.815	-41.219
4900	1214.187	3266.111	2231.732	5068.456	364.697	3858.932	-41.136
5000	1214.820	3290.647	2252.666	5189.907	355.526	3930.460	-41.060

3.589. Benzo[*j*]naphtho[8,1,2-*abc*]coronene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 75459-00-6
Point Group: C_s

Length: 16.55 Å
Width: 11.66 Å
Breadth: 3.886 Å
L/B Ratio: 1.419

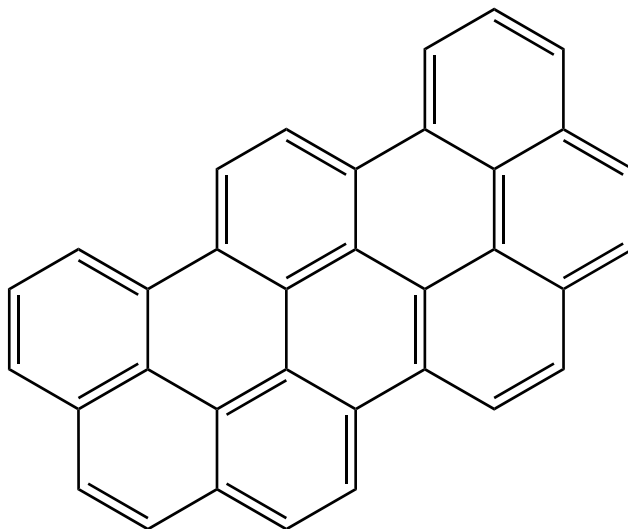
Cartesian coordinates:

C	2.3876	-2.9056	0.0000	C	0.4016	1.5876	0.0000	H	3.2933	-3.5316	0.0000
C	1.1492	-3.4701	0.0000	C	-3.3535	1.2260	0.0000	H	1.0299	-4.5596	0.0000
C	1.4295	-0.6691	0.0000	C	-4.5153	2.0088	0.0000	H	-1.4092	-4.3214	0.0000
C	2.5570	-1.4884	0.0000	C	-5.7690	1.4164	0.0000	H	-0.5102	4.8907	0.0000
C	-0.0231	-2.6544	0.0000	C	-5.8967	0.0309	0.0000	H	-2.7777	3.8575	0.0000
C	0.1215	-1.2506	0.0000	C	-3.4763	-0.1812	0.0000	H	3.9564	3.2053	0.0000
C	-1.3099	-3.2289	0.0000	C	-4.7591	-0.7773	0.0000	H	1.9338	4.6533	0.0000
C	-1.0325	-0.4280	0.0000	C	-4.8657	-2.2175	0.0000	H	-4.4140	3.1050	0.0000
C	-2.0330	1.8230	0.0000	C	-3.7664	-3.0008	0.0000	H	-6.6664	2.0441	0.0000
C	-0.9006	1.0057	0.0000	C	-2.4399	-2.4283	0.0000	H	-6.8915	-0.4288	0.0000
C	-0.6267	3.8009	0.0000	C	-2.3062	-1.0112	0.0000	H	-5.8707	-2.6552	0.0000
C	-1.8703	3.2337	0.0000	C	4.0111	0.5060	0.0000	H	-3.8516	-4.0936	0.0000
C	1.5683	0.7618	0.0000	C	3.8731	-0.8947	0.0000	H	4.9154	-2.7933	0.0000
C	2.8362	1.3461	0.0000	C	5.0352	-1.6991	0.0000	H	7.1815	-1.7629	0.0000
C	2.9470	2.7659	0.0000	C	6.2872	-1.1313	0.0000	H	7.4253	0.7116	0.0000
C	1.8392	3.5614	0.0000	C	6.4250	0.2666	0.0000	H	5.4040	2.1645	0.0000
C	0.5369	2.9870	0.0000	C	5.3078	1.0679	0.0000				

Table 3.589: Table of thermodynamic data as a function of temperature for Benzo[*j*]naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.808	479.624	479.624	∞
100	120.545	368.387	874.008	-50.562	506.500	553.480	-289.102
200	253.363	490.581	651.450	-32.174	492.252	606.153	-158.308
250	329.141	555.211	625.698	-17.622	485.572	635.399	-132.757
298.15	402.586	619.482	619.482	0.000	479.624	664.810	-116.470
300	405.370	621.981	619.490	0.747	479.403	665.957	-115.951
350	478.583	690.023	624.696	22.864	473.914	697.496	-104.093
400	546.533	758.432	637.138	48.517	469.143	729.759	-95.295
450	608.159	826.426	654.400	77.412	464.998	762.590	-88.517
500	663.280	893.411	674.962	109.224	461.382	795.879	-83.143
600	755.642	1022.843	722.250	180.356	455.430	863.367	-75.161
700	828.399	1145.008	774.009	259.700	450.988	931.735	-69.525
800	886.381	1259.552	827.621	345.545	447.895	1000.627	-65.333
900	933.285	1366.755	881.635	436.608	445.976	1069.826	-62.090
1000	971.748	1467.142	935.221	531.921	445.075	1139.199	-59.504
1100	1003.651	1561.302	987.902	630.739	444.985	1208.634	-57.392
1200	1030.363	1649.809	1039.411	732.479	445.567	1278.024	-55.630
1300	1052.909	1733.198	1089.603	836.673	446.627	1347.359	-54.136
1400	1072.075	1811.947	1138.413	942.948	448.030	1416.602	-52.853
1500	1088.471	1886.486	1185.822	1050.996	449.698	1485.739	-51.737
1600	1102.582	1957.196	1231.842	1160.566	451.490	1554.748	-50.756
1700	1114.793	2024.415	1276.503	1271.449	453.333	1623.616	-49.887
1800	1125.416	2088.442	1319.847	1383.472	455.146	1692.451	-49.113
1900	1134.703	2149.545	1361.919	1496.488	456.900	1761.124	-48.416
2000	1142.859	2207.959	1402.772	1610.375	458.541	1829.739	-47.787
2100	1150.055	2263.897	1442.455	1725.028	459.980	1898.259	-47.216
2200	1156.430	2317.548	1481.021	1840.359	461.221	1966.716	-46.695
2300	1162.101	2369.081	1518.519	1956.291	462.262	2035.125	-46.218
2400	1167.164	2418.648	1554.999	2072.758	463.022	2103.432	-45.779
2500	1171.701	2466.388	1590.505	2189.706	463.520	2171.851	-45.377
2600	1175.779	2512.423	1625.084	2307.083	463.713	2240.113	-45.003
2700	1179.459	2556.868	1658.776	2424.848	463.610	2308.466	-44.659
2800	1182.788	2599.823	1691.622	2542.963	463.181	2376.849	-44.340
2900	1185.808	2641.382	1723.660	2661.396	462.394	2445.192	-44.042
3000	1188.557	2681.630	1754.925	2780.116	461.302	2513.602	-43.765
3100	1191.065	2720.644	1785.451	2899.099	459.813	2581.954	-43.505
3200	1193.358	2758.496	1815.270	3018.322	457.980	2650.454	-43.263
3300	1195.461	2795.250	1844.412	3137.764	455.782	2719.067	-43.038
3400	1197.393	2830.967	1872.906	3257.408	453.184	2787.641	-42.826
3500	1199.172	2865.703	1900.778	3377.238	450.196	2856.276	-42.627
3600	1200.814	2899.508	1928.053	3497.238	446.844	2925.114	-42.441
3700	1202.332	2932.430	1954.755	3617.397	443.091	2994.064	-42.268
3800	1203.738	2964.513	1980.907	3737.701	438.907	3063.055	-42.104
3900	1205.043	2995.797	2006.531	3858.141	434.341	3132.090	-41.949
4000	1206.256	3026.322	2031.645	3978.706	429.374	3201.422	-41.805
4100	1207.385	3056.122	2056.271	4099.389	423.965	3270.793	-41.670
4200	1208.438	3085.229	2080.424	4220.181	418.147	3340.291	-41.542
4300	1209.422	3113.676	2104.124	4341.074	411.904	3409.820	-41.420
4400	1210.342	3141.491	2127.386	4462.063	405.247	3479.611	-41.307
4500	1211.204	3168.701	2150.225	4583.141	398.195	3549.623	-41.202
4600	1212.012	3195.330	2172.656	4704.302	390.682	3619.816	-41.103
4700	1212.771	3221.404	2194.693	4825.542	382.730	3690.033	-41.009
4800	1213.485	3246.945	2216.350	4946.855	374.391	3760.556	-40.922
4900	1214.157	3271.973	2237.639	5068.237	365.577	3831.087	-40.839
5000	1214.790	3296.509	2258.572	5189.685	356.403	3902.029	-40.763

3.590. Benzo[*pqr*]dinaphtho[8,1,2-*bcd*:2',1',8'-*lmn*]perylene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 188-11-4
Point Group: C_{2v}

Length: 15.94 Å
Width: 10.41 Å
Breadth: 3.885 Å
L/B Ratio: 1.531

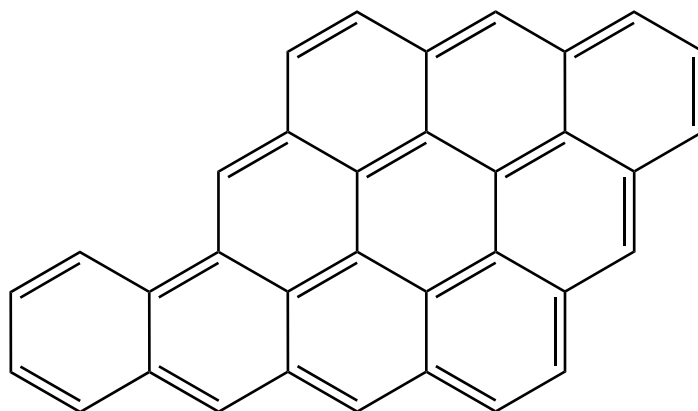
Cartesian coordinates:

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C	5.0036	-2.8156	0.0000	C	-1.4011	-1.6788	0.0000	H	6.7787	-1.5939	0.0000
C	5.6830	-1.6123	0.0000	C	-1.4218	0.7967	0.0000	H	6.7535	0.8544	0.0000
C	3.5611	-0.4205	0.0000	C	-0.7352	2.0178	0.0000	H	5.4907	2.9922	0.0000
C	4.9711	-0.4004	0.0000	C	-1.4700	3.2245	0.0000	H	3.3592	4.1973	0.0000
C	5.6574	0.8617	0.0000	C	-2.8432	3.2201	0.0000	H	0.8721	4.1836	0.0000
C	4.9682	2.0286	0.0000	C	-2.8424	0.7887	0.0000	H	-1.2297	-3.8293	0.0000
C	2.8344	0.8169	0.0000	C	-3.5528	2.0002	0.0000	H	1.2676	-3.8169	0.0000
C	3.5327	2.0355	0.0000	C	-4.9882	1.9790	0.0000	H	-0.9138	4.1747	0.0000
C	2.8110	3.2483	0.0000	C	-5.6658	0.8053	0.0000	H	-3.4009	4.1636	0.0000
C	1.4378	3.2390	0.0000	C	-3.5568	-0.4559	0.0000	H	-5.5202	2.9373	0.0000
C	1.4138	0.8108	0.0000	C	-4.9669	-0.4500	0.0000	H	-6.7617	0.7870	0.0000
C	0.7150	2.0250	0.0000	C	-5.6666	-1.6690	0.0000	H	-6.7624	-1.6617	0.0000
C	0.7091	-0.4468	0.0000	C	-4.9752	-2.8654	0.0000	H	-5.5215	-3.8145	0.0000
C	-0.6774	-2.8767	0.0000	C	-3.5792	-2.8771	0.0000	H	-3.0331	-3.8331	0.0000
C	0.7058	-2.8699	0.0000	C	-2.8575	-1.6875	0.0000				

Table 3.590: Table of thermodynamic data as a function of temperature for Benzo[*pqr*]dinaphtho[8,1,2-*bcd*:2',1',8'-*lmn*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-57.379	475.502	475.502	∞
100	118.729	358.261	861.327	-50.307	502.633	550.625	-287.611
200	252.109	479.347	639.721	-32.075	488.229	604.376	-157.844
250	328.148	543.726	614.040	-17.578	481.493	634.191	-132.504
298.15	401.778	607.839	607.839	0.000	475.502	664.159	-116.356
300	404.569	610.333	607.847	0.746	475.280	665.327	-115.841
350	477.930	678.263	613.044	22.827	469.754	697.452	-104.087
400	545.997	746.592	625.467	48.450	464.954	730.305	-95.366
450	607.719	814.529	642.707	77.320	460.784	763.730	-88.650
500	662.918	881.472	663.247	109.113	457.149	797.614	-83.324
600	755.399	1010.850	710.492	180.214	451.166	866.299	-75.416
700	828.241	1132.984	762.215	259.538	446.704	935.868	-69.834
800	886.284	1247.511	815.797	345.371	443.598	1005.964	-65.681
900	933.231	1354.705	869.786	436.427	441.672	1076.368	-62.469
1000	971.726	1455.088	923.352	531.736	440.768	1146.946	-59.909
1100	1003.651	1549.247	976.016	630.553	440.677	1217.587	-57.817
1200	1030.378	1637.755	1027.511	732.293	441.259	1288.182	-56.072
1300	1052.935	1721.145	1077.691	836.490	442.322	1358.722	-54.593
1400	1072.107	1799.896	1126.491	942.768	443.728	1429.170	-53.322
1500	1088.508	1874.438	1173.892	1050.820	445.399	1499.512	-52.217
1600	1102.621	1945.150	1219.904	1160.393	447.195	1569.726	-51.245
1700	1114.833	2012.371	1264.559	1271.280	449.042	1639.798	-50.384
1800	1125.456	2076.401	1307.897	1383.307	450.859	1709.838	-49.617
1900	1134.742	2137.506	1349.965	1496.327	452.617	1779.714	-48.927
2000	1142.898	2195.922	1390.813	1610.218	454.262	1849.533	-48.304
2100	1150.093	2251.862	1430.493	1724.875	455.704	1919.257	-47.738
2200	1156.467	2305.515	1469.056	1840.209	456.949	1988.918	-47.222
2300	1162.136	2357.049	1506.551	1956.145	457.994	2058.530	-46.750
2400	1167.197	2406.618	1543.028	2072.616	458.758	2128.039	-46.315
2500	1171.733	2454.359	1578.532	2189.567	459.258	2197.661	-45.917
2600	1175.810	2500.396	1613.109	2306.947	459.455	2267.126	-45.546
2700	1179.488	2544.842	1646.799	2424.715	459.355	2336.682	-45.205
2800	1182.816	2587.798	1679.643	2542.833	458.929	2406.268	-44.889
2900	1185.835	2629.358	1711.679	2661.268	458.144	2475.813	-44.593
3000	1188.583	2669.607	1742.943	2779.991	457.055	2545.425	-44.319
3100	1191.089	2708.622	1773.468	2898.977	455.568	2614.980	-44.061
3200	1193.382	2746.474	1803.286	3018.202	453.737	2684.682	-43.822
3300	1195.483	2783.229	1832.427	3137.647	451.542	2754.498	-43.599
3400	1197.414	2818.947	1860.919	3257.293	448.946	2824.273	-43.389
3500	1199.192	2853.683	1888.790	3377.124	445.960	2894.110	-43.191
3600	1200.833	2887.488	1916.064	3497.127	442.610	2964.150	-43.008
3700	1202.350	2920.411	1942.766	3617.287	438.859	3034.302	-42.836
3800	1203.756	2952.494	1968.917	3737.593	434.677	3104.495	-42.673
3900	1205.060	2983.779	1994.540	3858.035	430.112	3174.731	-42.520
4000	1206.272	3014.304	2019.654	3978.602	425.148	3245.266	-42.378
4100	1207.401	3044.104	2044.279	4099.286	419.740	3315.839	-42.243
4200	1208.453	3073.213	2068.432	4220.080	413.923	3386.538	-42.117
4300	1209.436	3101.660	2092.131	4340.975	407.682	3457.269	-41.997
4400	1210.356	3129.475	2115.392	4461.965	401.026	3528.261	-41.885
4500	1211.217	3156.685	2138.231	4583.044	393.975	3599.475	-41.781
4600	1212.025	3183.315	2160.661	4704.206	386.464	3670.869	-41.683
4700	1212.784	3209.389	2182.698	4825.447	378.513	3742.288	-41.590
4800	1213.497	3234.930	2204.355	4946.762	370.175	3814.012	-41.504
4900	1214.169	3259.958	2225.643	5068.145	361.363	3885.745	-41.422
5000	1214.802	3284.494	2246.575	5189.594	352.190	3957.888	-41.347

3.591. Naphtho[3,2,1,8,7-*defgh*]pyranthrene



Formula: C₃₄H₁₆
Mass: 424.491 g/mol
CAS Number: 128345-71-1
Point Group: C_s

Length: 17.98 Å
Width: 11.69 Å
Breadth: 3.886 Å
L/B Ratio: 1.539

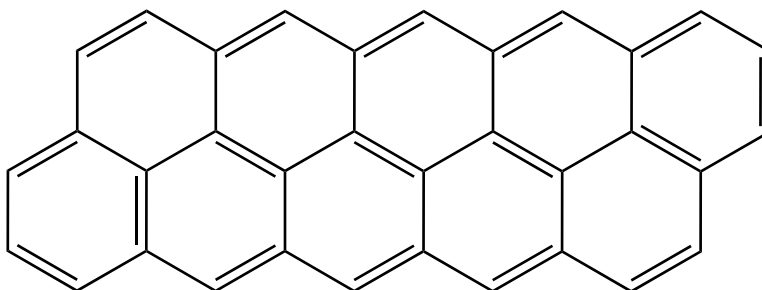
Cartesian coordinates:

C	6.4708	-1.5081	0.0000	C	2.2163	-2.0443	0.0000	H	7.1470	-2.3692	0.0000
C	7.0135	-0.2044	0.0000	C	2.8074	-0.7485	0.0000	H	8.1011	-0.0784	0.0000
C	6.1864	0.8872	0.0000	C	1.9818	0.3867	0.0000	H	6.6003	1.9021	0.0000
C	5.1132	-1.6909	0.0000	C	-4.4904	0.9173	0.0000	H	4.6746	-2.7006	0.0000
C	4.2315	-0.5795	0.0000	C	-5.8752	0.7475	0.0000	H	4.3661	2.8567	0.0000
C	4.7750	0.7222	0.0000	C	-6.4268	-0.5330	0.0000	H	2.1258	3.8439	0.0000
C	3.9191	1.8547	0.0000	C	-5.6175	-1.6570	0.0000	H	-0.1220	4.8398	0.0000
C	2.5506	1.7022	0.0000	C	-3.6534	-0.2274	0.0000	H	-2.5797	4.5659	0.0000
C	1.6707	2.8456	0.0000	C	-4.2192	-1.5237	0.0000	H	-4.5554	3.0979	0.0000
C	0.3180	2.6987	0.0000	C	-3.3578	-2.6665	0.0000	H	2.8886	-2.9173	0.0000
C	-0.5782	3.8428	0.0000	C	-2.2357	-0.0727	0.0000	H	-6.5315	1.6251	0.0000
C	-1.9151	3.6940	0.0000	C	-1.4068	-1.2097	0.0000	H	-7.5160	-0.6486	0.0000
C	-2.5364	2.3805	0.0000	C	-1.9961	-2.5225	0.0000	H	-6.0634	-2.6581	0.0000
C	-3.8910	2.2249	0.0000	C	-1.1035	-3.6664	0.0000	H	-3.8137	-3.6642	0.0000
C	-1.6648	1.2269	0.0000	C	0.2353	-3.5173	0.0000	H	-1.5597	-4.6632	0.0000
C	-0.2774	1.3789	0.0000	C	0.8533	-2.2053	0.0000	H	0.9000	-4.3890	0.0000
C	0.5641	0.2362	0.0000	C	-0.0030	-1.0553	0.0000				

Table 3.591: Table of thermodynamic data as a function of temperature for Naphtho[3,2,1,8,7-*defgh*]pyranthrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-57.729	527.803	527.803	∞
100	119.346	364.003	870.617	-50.661	554.580	601.998	-314.445
200	254.083	486.009	647.454	-32.289	540.317	655.131	-171.099
250	330.374	550.862	621.608	-17.686	533.687	684.601	-143.037
298.15	404.004	615.369	615.369	0.000	527.803	714.216	-125.125
300	406.791	617.877	615.377	0.750	527.585	715.370	-124.554
350	479.978	686.138	620.601	22.938	522.168	747.109	-111.498
400	547.800	754.725	633.081	48.658	517.463	779.561	-101.798
450	609.269	822.860	650.389	77.612	513.377	812.574	-94.319
500	664.244	889.954	671.002	109.476	509.814	846.039	-88.383
600	756.387	1019.541	718.387	180.692	503.946	913.864	-79.557
700	829.022	1141.811	770.234	260.104	499.571	982.557	-73.318
800	886.942	1256.433	823.924	346.007	496.537	1051.765	-68.672
900	933.813	1363.700	878.005	437.125	494.672	1121.272	-65.076
1000	972.256	1464.141	931.651	532.490	493.823	1190.948	-62.207
1100	1004.141	1558.349	984.387	631.358	493.784	1260.681	-59.864
1200	1030.835	1646.898	1035.944	733.145	494.413	1330.364	-57.908
1300	1053.362	1730.324	1086.180	837.386	495.520	1399.988	-56.251
1400	1072.506	1809.106	1135.030	943.705	496.967	1469.517	-54.827
1500	1088.881	1883.674	1182.477	1051.796	498.677	1538.937	-53.589
1600	1102.970	1954.409	1228.531	1161.405	500.509	1608.225	-52.502
1700	1115.159	2021.651	1273.224	1272.326	502.390	1677.370	-51.538
1800	1125.760	2085.699	1316.596	1384.384	504.238	1746.481	-50.681
1900	1135.027	2146.819	1358.696	1497.434	506.025	1815.427	-49.909
2000	1143.164	2205.250	1399.574	1611.352	507.698	1884.314	-49.212
2100	1150.342	2261.202	1439.281	1726.035	509.166	1953.105	-48.580
2200	1156.700	2314.866	1477.869	1841.393	510.435	2021.831	-48.003
2300	1162.355	2366.410	1515.388	1957.351	511.503	2090.507	-47.476
2400	1167.403	2415.988	1551.887	2073.844	512.287	2159.080	-46.990
2500	1171.926	2463.737	1587.412	2190.814	512.808	2227.764	-46.546
2600	1175.992	2509.782	1622.007	2308.214	513.023	2296.291	-46.132
2700	1179.659	2554.234	1655.716	2425.999	512.941	2364.909	-45.751
2800	1182.977	2597.196	1688.577	2544.134	512.531	2433.554	-45.398
2900	1185.988	2638.762	1720.629	2662.585	511.762	2502.160	-45.068
3000	1188.727	2679.016	1751.908	2781.322	510.688	2570.831	-44.761
3100	1191.225	2718.035	1782.448	2900.322	509.215	2639.445	-44.473
3200	1193.511	2755.892	1812.279	3019.560	507.398	2708.205	-44.206
3300	1195.606	2792.651	1841.433	3139.018	505.215	2777.079	-43.957
3400	1197.531	2828.372	1869.938	3258.676	502.631	2845.912	-43.721
3500	1199.303	2863.111	1897.820	3378.519	499.656	2914.806	-43.500
3600	1200.939	2896.920	1925.106	3498.532	496.317	2983.903	-43.294
3700	1202.451	2929.845	1951.818	3618.702	492.576	3053.112	-43.101
3800	1203.851	2961.931	1977.979	3739.018	488.404	3122.361	-42.919
3900	1205.151	2993.219	2003.612	3859.469	483.849	3191.654	-42.747
4000	1206.359	3023.746	2028.735	3980.046	478.893	3261.244	-42.587
4100	1207.484	3053.548	2053.368	4100.738	473.494	3330.872	-42.435
4200	1208.533	3082.659	2077.530	4221.540	467.685	3400.627	-42.292
4300	1209.513	3111.108	2101.237	4342.443	461.452	3470.414	-42.156
4400	1210.429	3138.924	2124.506	4463.440	454.804	3540.461	-42.030
4500	1211.288	3166.136	2147.352	4584.527	447.760	3610.730	-41.911
4600	1212.093	3192.767	2169.790	4705.696	440.256	3681.179	-41.800
4700	1212.849	3218.843	2191.834	4826.944	432.311	3751.652	-41.694
4800	1213.560	3244.385	2213.497	4948.264	423.980	3822.431	-41.596
4900	1214.229	3269.415	2234.792	5069.654	415.174	3893.218	-41.501
5000	1214.859	3293.952	2255.730	5191.109	406.006	3964.416	-41.415

3.592. peri-Pentacenopentacene



Formula: $C_{34}H_{16}$
Mass: 424.491 g/mol
CAS Number: 74335-56-1
Point Group: C_{2h}

Length: 17.73 Å
Width: 9.554 Å
Breadth: 3.885 Å
L/B Ratio: 1.856

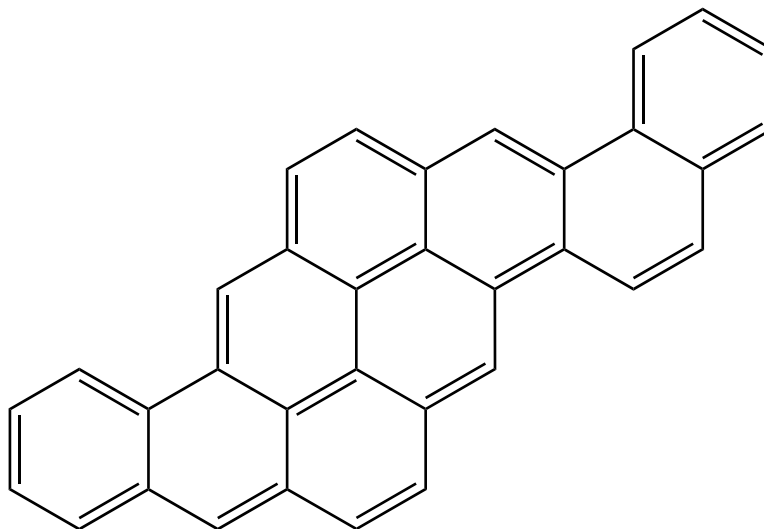
Cartesian coordinates:

C	6.7118	-0.1349	0.0000	C	-4.3890	-1.4614	0.0000	H	7.6300	-0.7330	0.0000
C	6.8071	1.2766	0.0000	C	-3.2228	-2.2431	0.0000	H	7.8010	1.7367	0.0000
C	5.6848	2.0568	0.0000	C	-3.0219	0.5680	0.0000	H	5.7612	3.1501	0.0000
C	4.3890	1.4614	0.0000	C	-1.8601	-0.2224	0.0000	H	3.3078	3.3367	0.0000
C	3.2228	2.2430	0.0000	C	-1.9629	-1.6455	0.0000	H	0.8565	3.5196	0.0000
C	1.9629	1.6455	0.0000	C	-0.7680	-2.4261	0.0000	H	-1.5931	3.7009	0.0000
C	0.7680	2.4261	0.0000	C	-0.5765	0.3943	0.0000	H	-4.0430	3.8781	0.0000
C	-0.4702	1.8287	0.0000	C	0.5766	-0.3942	0.0000	H	-6.2652	2.7872	0.0000
C	-1.6830	2.6075	0.0000	C	0.4702	-1.8286	0.0000	H	-7.6301	0.7327	0.0000
C	-2.9077	2.0105	0.0000	C	1.6829	-2.6074	0.0000	H	-7.8011	-1.7366	0.0000
C	-4.1356	2.7857	0.0000	C	1.8602	0.2224	0.0000	H	-5.7610	-3.1502	0.0000
C	-5.3440	2.1929	0.0000	C	3.0219	-0.5680	0.0000	H	-3.3075	-3.3368	0.0000
C	-5.4805	0.7486	0.0000	C	2.9077	-2.0105	0.0000	H	-0.8562	-3.5196	0.0000
C	-6.7117	0.1349	0.0000	C	4.1355	-2.7857	0.0000	H	1.5932	-3.7009	0.0000
C	-6.8071	-1.2767	0.0000	C	5.3439	-2.1929	0.0000	H	4.0430	-3.8781	0.0000
C	-5.6848	-2.0569	0.0000	C	5.4804	-0.7486	0.0000	H	6.2651	-2.7872	0.0000
C	-4.2898	-0.0465	0.0000	C	4.2899	0.0465	0.0000				

Table 3.592: Table of thermodynamic data as a function of temperature for peri-Pentacenopentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-57.618	557.259	557.259	∞
100	117.846	356.280	863.096	-50.682	584.016	632.206	-330.224
200	254.267	477.660	639.608	-32.390	569.672	686.156	-179.202
250	331.464	542.656	613.672	-17.754	563.075	716.040	-149.605
298.15	405.674	607.410	607.410	0.000	557.259	746.045	-130.701
300	408.478	609.928	607.418	0.753	557.044	747.214	-130.099
350	482.000	678.477	612.663	23.035	551.720	779.343	-116.308
400	549.975	747.346	625.196	48.860	547.121	812.171	-106.056
450	611.479	815.739	642.575	77.924	543.145	845.546	-98.146
500	666.414	883.065	663.268	109.898	539.691	879.361	-91.864
600	758.378	1013.033	710.828	181.323	534.032	947.855	-82.516
700	830.793	1135.593	762.846	260.923	529.846	1017.184	-75.902
800	888.504	1250.438	816.697	346.993	526.978	1087.002	-70.972
900	935.191	1357.878	870.926	438.257	525.260	1157.100	-67.155
1000	973.475	1458.456	924.704	533.752	524.541	1227.351	-64.109
1100	1005.224	1552.773	977.560	632.735	524.616	1297.647	-61.619
1200	1031.801	1641.412	1029.225	734.624	525.348	1367.882	-59.541
1300	1054.227	1724.910	1079.559	838.957	526.546	1438.051	-57.780
1400	1073.284	1803.753	1128.498	945.358	528.075	1508.118	-56.267
1500	1089.584	1878.372	1176.024	1053.522	529.859	1578.071	-54.952
1600	1103.607	1949.151	1222.152	1163.199	531.758	1647.887	-53.797
1700	1115.738	2016.430	1266.912	1274.180	533.700	1717.556	-52.773
1800	1126.289	2080.509	1310.346	1386.294	535.603	1787.188	-51.862
1900	1135.511	2141.657	1352.502	1499.394	537.441	1856.651	-51.042
2000	1143.609	2200.111	1393.432	1613.359	539.160	1926.053	-50.302
2100	1150.752	2256.085	1433.188	1728.084	540.671	1995.357	-49.631
2200	1157.079	2309.767	1471.820	1843.482	541.979	2064.593	-49.019
2300	1162.705	2361.327	1509.381	1959.476	543.084	2133.779	-48.459
2400	1167.728	2410.920	1545.919	2076.003	543.902	2202.859	-47.943
2500	1172.229	2458.682	1581.480	2193.005	544.454	2272.050	-47.471
2600	1176.274	2504.737	1616.109	2310.433	544.699	2341.082	-47.032
2700	1179.923	2549.200	1649.850	2428.246	544.643	2410.203	-46.627
2800	1183.224	2592.172	1682.741	2546.406	544.260	2479.352	-46.252
2900	1186.220	2633.746	1714.821	2664.881	543.514	2548.459	-45.902
3000	1188.945	2674.007	1746.127	2783.641	542.463	2617.631	-45.576
3100	1191.431	2713.033	1776.691	2902.662	541.011	2686.746	-45.270
3200	1193.704	2750.896	1806.546	3021.920	539.214	2756.006	-44.986
3300	1195.789	2787.661	1835.723	3141.397	537.050	2825.379	-44.721
3400	1197.704	2823.388	1864.249	3261.073	534.484	2894.711	-44.471
3500	1199.467	2858.132	1892.151	3380.932	531.525	2964.103	-44.236
3600	1201.094	2891.945	1919.456	3500.961	528.203	3033.698	-44.017
3700	1202.598	2924.875	1946.186	3621.147	524.476	3103.404	-43.811
3800	1203.992	2956.964	1972.365	3741.477	520.319	3173.150	-43.617
3900	1205.285	2988.256	1998.014	3861.942	515.777	3242.939	-43.433
4000	1206.487	3018.786	2023.153	3982.531	510.835	3313.026	-43.263
4100	1207.606	3048.591	2047.802	4103.237	505.448	3383.150	-43.101
4200	1208.649	3077.704	2071.978	4224.050	499.651	3453.400	-42.948
4300	1209.624	3106.156	2095.699	4344.964	493.429	3523.682	-42.803
4400	1210.536	3133.975	2118.982	4465.973	486.792	3594.225	-42.668
4500	1211.389	3161.189	2141.840	4587.069	479.759	3664.988	-42.541
4600	1212.190	3187.823	2164.291	4708.249	472.264	3735.932	-42.422
4700	1212.942	3213.901	2186.346	4829.506	464.329	3806.900	-42.308
4800	1213.649	3239.445	2208.021	4950.836	456.007	3878.172	-42.202
4900	1214.315	3264.476	2229.326	5072.234	447.209	3949.453	-42.101
5000	1214.942	3289.015	2250.276	5193.697	438.051	4021.145	-42.008

3.593. Benzo[*a*]pyranthrene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 191-12-8
Point Group: C_s

Length: 20.15 Å
Width: 10.44 Å
Breadth: 3.885 Å
L/B Ratio: 1.930

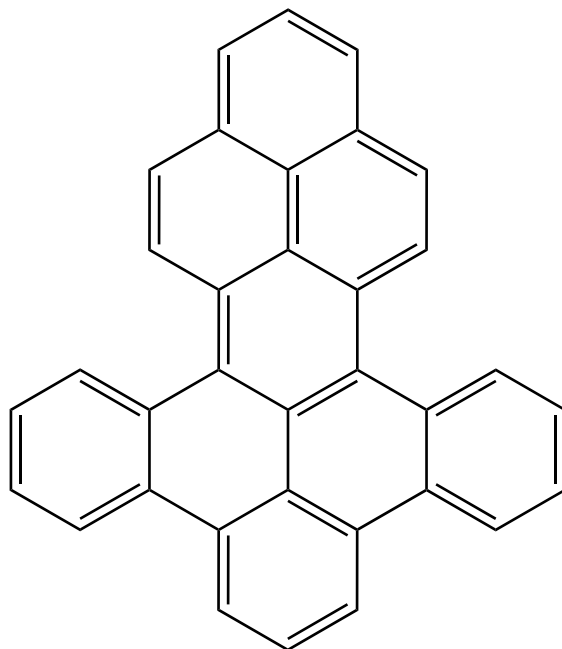
Cartesian coordinates:

C	6.9317	-1.8534	0.0000	C	-0.8451	-0.4714	0.0000	H	7.5216	1.5062	0.0000
C	7.6451	-0.6386	0.0000	C	-1.5888	-1.6900	0.0000	H	4.9870	-2.7893	0.0000
C	6.9723	0.5578	0.0000	C	-0.8687	-2.9464	0.0000	H	5.4381	2.7584	0.0000
C	5.5590	-1.8487	0.0000	C	0.4786	-2.9843	0.0000	H	3.3493	4.0412	0.0000
C	4.8409	-0.6292	0.0000	C	1.2645	-1.7686	0.0000	H	0.8745	4.1061	0.0000
C	5.5556	0.5843	0.0000	C	0.5802	-0.5148	0.0000	H	-1.2849	2.9266	0.0000
C	4.8568	1.8280	0.0000	C	-3.6599	-0.4163	0.0000	H	3.1848	-2.7582	0.0000
C	3.4875	1.8611	0.0000	C	-2.9435	0.7901	0.0000	H	-3.5534	-2.5821	0.0000
C	2.7605	3.1164	0.0000	C	-3.6577	2.0326	0.0000	H	-1.4594	-3.8699	0.0000
C	1.4147	3.1522	0.0000	C	-5.0131	2.0659	0.0000	H	1.0175	-3.9388	0.0000
C	0.6270	1.9350	0.0000	C	-5.1053	-0.3868	0.0000	H	-3.0672	2.9617	0.0000
C	-0.7453	1.9659	0.0000	C	-5.7728	0.8510	0.0000	H	-5.5536	3.0194	0.0000
C	1.3176	0.6787	0.0000	C	-7.1857	0.8855	0.0000	H	-7.6954	1.8557	0.0000
C	2.6424	-1.7988	0.0000	C	-7.9084	-0.2839	0.0000	H	-9.0030	-0.2591	0.0000
C	3.4010	-0.6027	0.0000	C	-7.2450	-1.5239	0.0000	H	-7.8319	-2.4483	0.0000
C	2.7381	0.6354	0.0000	C	-5.8714	-1.5747	0.0000	H	-5.3424	-2.5399	0.0000
C	-1.5129	0.7664	0.0000	H	7.4823	-2.7997	0.0000				
C	-2.9652	-1.6502	0.0000	H	8.7398	-0.6596	0.0000				

Table 3.593: Table of thermodynamic data as a function of temperature for Benzo[*a*]pyranthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	
0	0.0	0.0	∞	-61.042	532.974	532.974	∞
100	131.040	379.523	911.835	-53.231	562.649	618.588	-323.110
200	266.575	509.760	678.099	-33.668	546.882	680.830	-177.811
250	344.380	577.550	651.173	-18.406	539.516	715.168	-149.423
298.15	419.914	644.684	644.684	0.000	532.974	749.609	-131.326
300	422.778	647.290	644.692	0.779	532.733	750.951	-130.749
350	498.051	718.173	650.118	23.819	526.717	787.810	-117.572
400	567.850	789.304	663.072	50.493	521.510	825.463	-107.792
450	631.106	859.905	681.028	80.495	517.011	863.733	-100.257
500	687.669	929.384	702.401	113.491	513.118	902.496	-94.281
600	782.511	1063.489	751.506	187.189	506.803	980.998	-85.402
700	857.416	1189.960	805.203	269.330	502.219	1060.424	-79.128
800	917.343	1308.507	860.789	358.175	499.173	1140.380	-74.458
900	966.033	1419.462	916.767	452.425	497.467	1220.627	-70.842
1000	1006.131	1523.385	972.289	551.096	496.920	1301.017	-67.957
1100	1039.519	1620.892	1026.867	653.428	497.305	1381.427	-65.597
1200	1067.569	1712.580	1080.228	758.822	498.463	1461.745	-63.627
1300	1091.312	1798.994	1132.226	866.798	500.185	1541.955	-61.955
1400	1111.544	1880.629	1182.795	976.968	502.318	1622.021	-60.517
1500	1128.888	1957.924	1231.917	1089.011	504.773	1701.926	-59.265
1600	1143.840	2031.270	1279.604	1202.666	507.399	1781.649	-58.164
1700	1156.799	2101.013	1325.888	1317.713	510.112	1861.175	-57.186
1800	1168.085	2167.460	1370.811	1433.970	512.825	1940.620	-56.314
1900	1177.963	2230.886	1414.421	1551.283	515.504	2019.850	-55.528
2000	1186.646	2291.533	1456.772	1669.523	518.088	2098.974	-54.818
2100	1194.313	2349.619	1497.915	1788.578	520.484	2177.955	-54.173
2200	1201.110	2405.339	1537.904	1908.356	522.692	2256.828	-53.583
2300	1207.160	2458.866	1576.790	2028.776	524.711	2335.606	-53.042
2400	1212.564	2510.359	1614.623	2149.767	526.453	2414.241	-52.544
2500	1217.409	2559.958	1651.450	2271.270	527.936	2492.949	-52.086
2600	1221.767	2607.792	1687.318	2393.232	529.117	2571.458	-51.660
2700	1225.699	2653.977	1722.270	2515.609	530.001	2650.020	-51.267
2800	1229.258	2698.618	1756.347	2638.360	530.559	2728.578	-50.901
2900	1232.488	2741.812	1789.588	2761.450	530.755	2807.059	-50.560
3000	1235.428	2783.645	1822.029	2884.848	530.644	2885.571	-50.241
3100	1238.111	2824.199	1853.707	3008.527	530.131	2963.997	-49.942
3200	1240.566	2863.547	1884.652	3132.462	529.269	3042.536	-49.663
3300	1242.817	2901.756	1914.897	3256.633	528.035	3121.159	-49.403
3400	1244.885	2938.889	1944.471	3381.020	526.396	3199.714	-49.157
3500	1246.790	2975.003	1973.402	3505.605	524.358	3278.302	-48.925
3600	1248.548	3010.151	2001.714	3630.373	521.949	3357.064	-48.709
3700	1250.174	3044.382	2029.434	3755.310	519.130	3435.916	-48.505
3800	1251.680	3077.743	2056.584	3880.404	515.871	3514.779	-48.313
3900	1253.078	3110.274	2083.186	4005.642	512.221	3593.665	-48.131
4000	1254.378	3142.016	2109.262	4131.016	508.160	3672.825	-47.961
4100	1255.588	3173.005	2134.830	4256.515	503.646	3752.000	-47.800
4200	1256.717	3203.275	2159.910	4382.131	498.713	3831.279	-47.648
4300	1257.771	3232.859	2184.520	4507.856	493.344	3910.569	-47.503
4400	1258.757	3261.786	2208.676	4633.683	487.550	3990.101	-47.368
4500	1259.681	3290.084	2232.394	4759.605	481.350	4069.839	-47.240
4600	1260.548	3317.780	2255.689	4885.617	474.678	4149.733	-47.121
4700	1261.362	3344.898	2278.576	5011.713	467.553	4229.634	-47.006
4800	1262.127	3371.462	2301.069	5137.888	460.033	4309.823	-46.899
4900	1262.848	3397.494	2323.180	5264.137	452.026	4390.004	-46.797
5000	1263.527	3423.014	2344.923	5390.456	443.648	4470.584	-46.703

3.594. Tetrabenzo[*a,cd,flm*]perylene



Formula: $C_{34}H_{18}$
Mass: 426.507 g/mol
CAS Number: 109278-10-6
Point Group: C_2

Length: 15.88 Å
Width: 13.94 Å
Breadth: 5.495 Å
L/B Ratio: 1.139

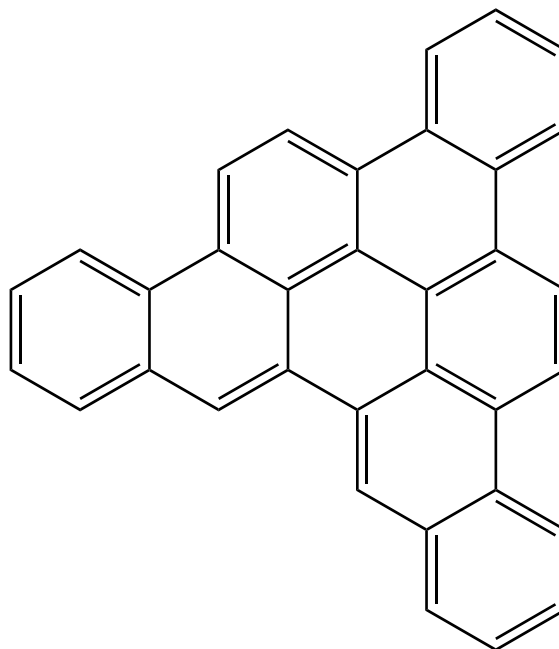
Cartesian coordinates:

C	4.4470	-1.1936	-0.0450	C	-3.3161	-2.2527	-0.9679	H	4.9948	2.1554	0.0394
C	5.1415	0.0056	-0.0183	C	-1.9673	-2.2813	-0.8743	H	-1.4210	3.1438	1.2627
C	4.4443	1.2029	0.0173	C	-1.2115	-1.1883	-0.3163	H	-3.8779	3.0758	1.4169
C	3.0455	1.2176	0.0092	C	-1.9139	-0.0034	0.0029	H	-6.0149	1.9740	0.8452
C	3.0484	-1.2116	-0.0211	C	2.3295	-2.4722	0.0487	H	-7.2460	-0.0024	-0.0169
C	2.3284	0.0022	-0.0034	C	0.9231	-2.4785	0.0660	H	-6.0095	-1.9800	-0.8676
C	-1.9730	2.2728	0.8835	C	0.2779	-3.7040	0.3227	H	-3.8691	-3.0863	-1.4158
C	-3.3223	2.2437	0.9693	C	0.9843	-4.8824	0.4636	H	-1.4136	-3.1545	-1.2459
C	-1.2140	1.1825	0.3242	C	2.3763	-4.8787	0.3591	H	-0.8162	-3.7354	0.4165
C	0.1838	-1.2300	-0.0921	C	3.0366	-3.6826	0.1657	H	0.4536	-5.8199	0.6595
C	0.8809	0.0004	0.0010	C	0.9164	2.4795	-0.0592	H	2.9375	-5.8144	0.4474
C	0.1807	1.2287	0.0976	C	2.3228	2.4766	-0.0486	H	4.1359	-3.6659	0.1150
C	-4.0658	1.1173	0.4752	C	3.0264	3.6898	-0.1594	H	4.1258	3.6760	-0.1137
C	-5.4637	1.1047	0.4693	C	2.3622	4.8857	-0.3408	H	2.9205	5.8236	-0.4232
C	-6.1509	-0.0029	-0.0120	C	0.9699	4.8863	-0.4408	H	0.4361	5.8239	-0.6275
C	-5.4606	-1.1111	-0.4872	C	0.2672	3.7050	-0.3063	H	-0.8272	3.7336	-0.3978
C	-3.3501	-0.0038	-0.0008	H	4.9993	-2.1450	-0.0718				
C	-4.0627	-1.1249	-0.4816	H	6.2364	0.0068	-0.0251				

Table 3.594: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,c,d,f,lm*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K_f</i>
0	0.0	0.0	∞	-60.944	586.041	586.041	∞
100	130.540	372.167	903.817	-53.165	615.782	672.456	-351.248
200	266.268	502.183	670.345	-33.632	599.985	735.447	-192.075
250	343.998	569.895	643.447	-18.388	592.601	770.166	-160.914
298.15	419.575	636.964	636.964	0.000	586.041	804.977	-141.026
300	422.443	639.568	636.972	0.779	585.799	806.334	-140.392
350	497.863	710.409	642.394	23.805	579.770	843.580	-125.895
400	567.841	781.527	655.342	50.474	574.558	881.621	-115.126
450	631.258	852.137	673.293	80.479	570.062	920.280	-106.821
500	687.942	921.638	694.664	113.487	566.180	959.431	-100.229
600	782.895	1055.805	743.773	187.219	559.899	1038.705	-90.425
700	857.784	1182.335	797.481	269.398	555.354	1118.896	-83.491
800	917.636	1300.927	853.082	358.276	552.341	1199.612	-78.325
900	966.235	1411.911	909.076	452.551	550.660	1280.616	-74.323
1000	1006.247	1515.851	964.613	551.238	550.129	1361.760	-71.130
1100	1039.563	1613.366	1019.204	653.578	550.522	1442.923	-68.517
1200	1067.556	1705.054	1072.576	758.973	551.681	1523.993	-66.336
1300	1091.258	1791.466	1124.584	866.946	553.399	1604.956	-64.487
1400	1111.460	1873.096	1175.161	977.109	555.525	1685.775	-62.896
1500	1128.783	1950.384	1224.289	1089.142	557.971	1766.434	-61.511
1600	1143.722	2023.723	1271.982	1202.786	560.586	1846.911	-60.294
1700	1156.672	2093.458	1318.270	1317.821	563.286	1927.192	-59.214
1800	1167.954	2159.899	1363.196	1434.065	565.986	2007.393	-58.252
1900	1177.830	2223.317	1406.809	1551.364	568.652	2087.379	-57.385
2000	1186.514	2283.957	1449.162	1669.591	571.223	2167.260	-56.602
2100	1194.183	2342.037	1490.307	1788.633	573.605	2246.999	-55.890
2200	1200.983	2397.750	1530.296	1908.398	575.801	2326.631	-55.240
2300	1207.036	2451.272	1569.183	2028.805	577.807	2406.169	-54.645
2400	1212.444	2502.760	1607.016	2149.784	579.537	2485.563	-54.096
2500	1217.293	2552.354	1643.844	2271.275	581.008	2565.031	-53.592
2600	1221.656	2600.184	1679.712	2393.227	582.178	2644.301	-53.124
2700	1225.592	2646.364	1714.663	2515.592	583.051	2723.624	-52.691
2800	1229.155	2691.002	1748.740	2638.333	583.599	2802.944	-52.288
2900	1232.390	2734.192	1781.981	2761.413	583.784	2882.186	-51.913
3000	1235.334	2776.022	1814.422	2884.801	583.664	2961.461	-51.563
3100	1238.022	2816.573	1846.098	3008.471	583.142	3040.648	-51.234
3200	1240.480	2855.918	1877.044	3132.398	582.271	3119.951	-50.927
3300	1242.734	2894.125	1907.288	3256.560	581.029	3199.336	-50.640
3400	1244.806	2931.255	1936.861	3380.938	579.381	3278.655	-50.369
3500	1246.715	2967.367	1965.791	3505.516	577.336	3358.006	-50.114
3600	1248.476	3002.513	1994.103	3630.276	574.919	3437.532	-49.876
3700	1250.105	3036.742	2021.822	3755.207	572.093	3517.148	-49.652
3800	1251.614	3070.101	2048.971	3880.293	568.827	3596.775	-49.440
3900	1253.014	3102.630	2075.572	4005.526	565.171	3676.425	-49.239
4000	1254.316	3134.371	2101.647	4130.893	561.104	3756.350	-49.052
4100	1255.529	3165.358	2127.215	4256.386	556.584	3836.289	-48.874
4200	1256.660	3195.627	2152.294	4381.996	551.645	3916.333	-48.706
4300	1257.717	3225.209	2176.903	4507.716	546.270	3996.387	-48.545
4400	1258.705	3254.135	2201.058	4633.537	540.471	4076.685	-48.395
4500	1259.631	3282.432	2224.776	4759.454	534.265	4157.188	-48.254
4600	1260.499	3310.127	2248.070	4885.461	527.588	4237.847	-48.121
4700	1261.315	3337.244	2270.957	5011.552	520.459	4318.513	-47.994
4800	1262.082	3363.808	2293.449	5137.723	512.935	4399.468	-47.875
4900	1262.804	3389.838	2315.559	5263.967	504.923	4480.415	-47.761
5000	1263.485	3415.357	2337.301	5390.282	496.541	4561.760	-47.655

3.595. Dibenzo[*fgh,pqr*]trinaphthylene



Formula: $C_{34}H_{18}$
Mass: 426.507 g/mol
CAS Number: 110789-63-4
Point Group: C_{2v}

Length: 15.91 Å
Width: 14.12 Å
Breadth: 3.894 Å
L/B Ratio: 1.126

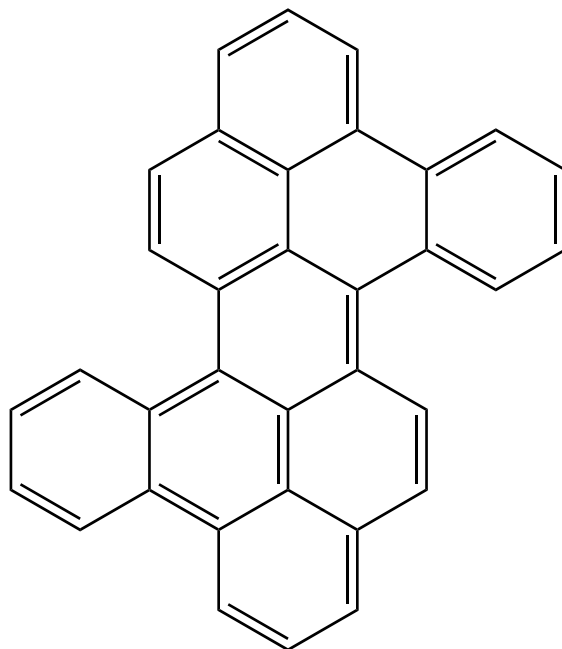
Cartesian coordinates:

C	-3.9445	3.5008	0.0000	C	1.3024	-5.8126	0.0000	H	-6.9903	1.9987	0.0000
C	-5.3120	3.3683	0.0000	C	1.8648	-4.5556	0.0000	H	-5.5565	-0.0412	0.0000
C	-5.8991	2.0892	0.0000	C	0.5775	1.5333	0.0000	H	-1.2576	3.4925	0.0000
C	-5.1097	0.9647	0.0000	C	1.1551	2.7740	0.0000	H	-4.4991	-1.4896	0.0000
C	-3.1166	2.3533	0.0000	C	2.8039	0.4938	0.0000	H	-3.0336	-3.5056	0.0000
C	-3.7000	1.0744	0.0000	C	1.4074	0.3572	0.0000	H	-1.9944	-4.9440	0.0000
C	-1.6954	2.4808	0.0000	C	0.8229	-0.9434	0.0000	H	-0.5348	-6.9574	0.0000
C	-2.8457	-0.0872	0.0000	C	1.6426	-2.0756	0.0000	H	1.9394	-6.7030	0.0000
C	-3.4026	-1.3909	0.0000	C	3.0513	-1.9138	0.0000	H	2.9588	-4.4347	0.0000
C	-2.5980	-2.4947	0.0000	C	3.6145	-0.6694	0.0000	H	0.5206	3.6753	0.0000
C	-1.1858	-2.3665	0.0000	C	2.5725	2.9383	0.0000	H	3.6835	-2.8149	0.0000
C	-0.6137	-1.0911	0.0000	C	3.4039	1.8049	0.0000	H	4.7081	-0.5427	0.0000
C	-0.8775	1.3837	0.0000	C	4.8065	1.9844	0.0000	H	5.4486	1.0904	0.0000
C	-1.4506	0.0633	0.0000	C	5.3505	3.2460	0.0000	H	6.4373	3.3794	0.0000
C	1.0558	-3.3999	0.0000	C	4.5154	4.3788	0.0000	H	4.9645	5.3774	0.0000
C	-0.3418	-3.5436	0.0000	C	3.1495	4.2303	0.0000	H	2.4928	5.1076	0.0000
C	-0.8987	-4.8398	0.0000	H	-3.4800	4.4934	0.0000				
C	-0.0923	-5.9560	0.0000	H	-5.9549	4.2546	0.0000				

Table 3.595: Table of thermodynamic data as a function of temperature for Dibenzo[*fgh,pqr*]trinaphthylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	Δ _{<i>f</i>} <i>H</i> ^o	Δ _{<i>f</i>} <i>G</i> ^o	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-61.758	531.366	531.366	∞
100	135.170	389.282	923.646	-53.436	560.836	615.799	-321.654
200	267.295	521.318	689.486	-33.633	545.309	676.944	-176.796
250	343.933	589.134	662.601	-18.367	537.948	710.703	-148.490
298.15	418.809	656.127	656.127	0.000	531.366	744.589	-130.446
300	421.655	658.726	656.135	0.777	531.123	745.910	-129.872
350	496.604	729.408	661.546	23.752	525.042	782.203	-116.735
400	566.293	800.337	674.463	50.349	519.759	819.298	-106.987
450	629.551	870.755	692.369	80.273	515.182	857.021	-99.478
500	686.169	940.072	713.685	113.194	511.212	895.246	-93.524
600	781.157	1073.916	762.668	186.749	504.754	972.694	-84.679
700	856.187	1200.189	816.245	268.760	500.042	1051.087	-78.431
800	916.210	1318.578	871.719	357.488	496.878	1130.028	-73.782
900	964.974	1429.403	927.594	451.628	495.062	1209.275	-70.183
1000	1005.138	1533.219	983.022	550.197	494.413	1288.676	-67.312
1100	1038.585	1630.634	1037.514	652.432	494.702	1368.108	-64.965
1200	1066.692	1722.243	1090.796	757.736	495.769	1447.455	-63.005
1300	1090.491	1808.589	1142.722	865.627	497.406	1526.702	-61.342
1400	1110.777	1890.165	1193.224	975.717	499.460	1605.812	-59.912
1500	1128.172	1967.409	1242.285	1087.687	501.841	1684.766	-58.668
1600	1143.172	2040.710	1289.915	1201.272	504.397	1763.542	-57.573
1700	1156.176	2110.414	1336.147	1316.255	507.046	1842.127	-56.601
1800	1167.504	2176.827	1381.021	1432.451	509.699	1920.633	-55.734
1900	1177.421	2240.223	1424.587	1549.708	512.322	1998.928	-54.953
2000	1186.140	2300.843	1466.895	1667.896	514.853	2077.119	-54.248
2100	1193.840	2358.905	1507.999	1786.902	517.200	2155.171	-53.606
2200	1200.668	2414.603	1547.951	1906.635	519.363	2233.117	-53.020
2300	1206.746	2468.112	1586.802	2027.011	521.338	2310.969	-52.483
2400	1212.176	2519.587	1624.603	2147.962	523.041	2388.680	-51.987
2500	1217.044	2569.171	1661.400	2269.428	524.486	2466.466	-51.533
2600	1221.424	2616.991	1697.239	2391.355	525.631	2544.055	-51.110
2700	1225.376	2663.163	1732.164	2513.698	526.482	2621.697	-50.719
2800	1228.954	2707.793	1766.216	2636.418	527.009	2699.338	-50.356
2900	1232.201	2750.976	1799.432	2759.478	527.175	2776.901	-50.016
3000	1235.157	2792.801	1831.851	2882.848	527.036	2854.498	-49.700
3100	1237.855	2833.346	1863.507	3006.501	526.497	2932.008	-49.403
3200	1240.323	2872.686	1894.432	3130.412	525.610	3009.633	-49.126
3300	1242.587	2910.888	1924.658	3254.559	524.353	3087.342	-48.868
3400	1244.667	2948.014	1954.213	3378.923	522.691	3164.985	-48.623
3500	1246.583	2984.122	1983.125	3503.486	520.632	3242.660	-48.393
3600	1248.351	3019.264	2011.421	3628.234	518.203	3320.511	-48.178
3700	1249.986	3053.490	2039.125	3753.152	515.365	3398.452	-47.977
3800	1251.501	3086.845	2066.259	3878.228	512.087	3476.404	-47.786
3900	1252.907	3119.372	2092.847	4003.449	508.419	3554.381	-47.605
4000	1254.215	3151.110	2118.908	4128.806	504.342	3632.631	-47.436
4100	1255.432	3182.095	2144.463	4254.289	499.812	3710.896	-47.276
4200	1256.567	3212.361	2169.531	4379.889	494.864	3789.266	-47.125
4300	1257.628	3241.942	2194.128	4505.600	489.480	3867.648	-46.982
4400	1258.620	3270.865	2218.272	4631.413	483.672	3946.272	-46.847
4500	1259.550	3299.161	2241.978	4757.322	477.458	4025.102	-46.721
4600	1260.421	3326.854	2265.262	4883.321	470.773	4104.088	-46.602
4700	1261.240	3353.970	2288.139	5009.404	463.637	4183.082	-46.489
4800	1262.010	3380.531	2310.621	5135.567	456.104	4262.365	-46.383
4900	1262.735	3406.560	2332.723	5261.805	448.086	4341.639	-46.281
5000	1263.419	3432.078	2354.455	5388.113	439.697	4421.312	-46.188

3.596. Tetrabenzo[*a,cd,j,lm*]perylene



Formula: $C_{34}H_{18}$
Mass: 426.507 g/mol
CAS Number: 191-53-7
Point Group: C_2

Length: 14.35 Å
Width: 11.29 Å
Breadth: 6.087 Å
L/B Ratio: 1.271

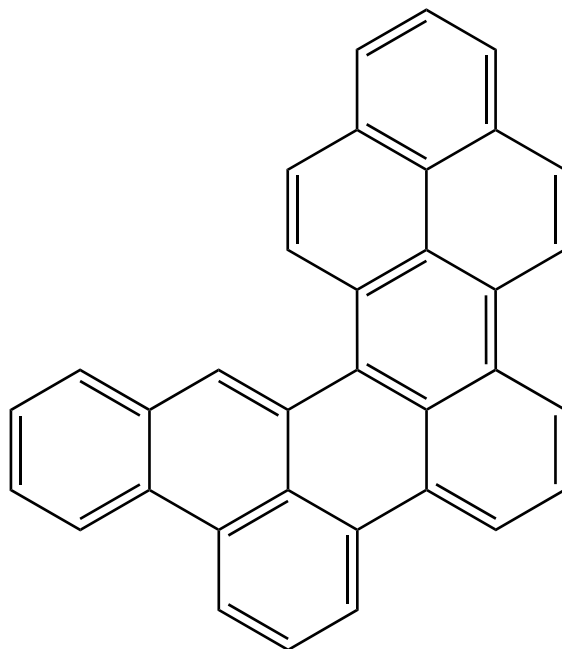
Cartesian coordinates:

C	4.9494	-1.1235	0.4691	C	-3.7289	0.5055	0.2001	H	3.8877	-4.2852	1.1419
C	5.0067	-2.4716	0.8139	C	-4.9495	1.1231	0.4694	H	1.4591	-4.4441	0.9663
C	3.8458	-3.2215	0.8819	C	-5.0070	2.4712	0.8142	H	-0.7214	-3.4037	0.5114
C	2.6054	-2.6209	0.6227	C	-3.8462	3.2213	0.8818	H	-1.4208	-3.2684	-1.1911
C	1.3912	-3.3833	0.6985	C	-2.5321	1.2510	0.2963	H	-3.5048	-4.4454	-1.7675
C	0.1966	-2.8027	0.4515	C	-2.6057	2.6210	0.6223	H	-5.7143	-3.3902	-1.3080
C	0.0724	-1.4021	0.1385	C	-1.3917	3.3835	0.6978	H	-5.8059	-1.0850	-0.3664
C	1.2519	-0.6165	0.1049	C	-0.1970	2.8030	0.4509	H	-5.8755	0.5329	0.3934
C	1.1822	0.7853	-0.0649	C	-0.0724	1.4024	0.1383	H	-5.9755	2.9364	1.0248
C	3.7289	-0.5058	0.1998	C	-1.2520	0.6168	0.1048	H	-3.8882	4.2852	1.1412
C	2.5319	-1.2510	0.2965	C	3.6585	0.8792	-0.2353	H	-1.4597	4.4445	0.9648
C	-1.1823	-0.7850	-0.0647	C	2.4075	1.5015	-0.4082	H	0.7207	3.4046	0.5101
C	-3.6584	-0.8795	-0.2350	C	2.3860	2.7825	-0.9903	H	1.4216	3.2697	-1.1896
C	-2.4073	-1.5015	-0.4079	C	3.5522	3.4493	-1.3149	H	3.5059	4.4462	-1.7655
C	-2.3854	-2.7820	-0.9909	C	4.7907	2.8539	-1.0696	H	5.7150	3.3901	-1.3070
C	-3.5515	-3.4490	-1.3159	C	4.8381	1.5783	-0.5430	H	5.8060	1.0844	-0.3662
C	-4.7901	-2.8541	-1.0700	H	5.8755	-0.5334	0.3930				
C	-4.8378	-1.5788	-0.5429	H	5.9751	-2.9369	1.0248				

Table 3.596: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,c,d,j,lm*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-61.030	575.059	575.059	∞
100	130.992	370.820	903.446	-53.263	604.703	661.512	-345.531
200	266.785	501.213	669.589	-33.675	588.960	724.617	-189.247
250	344.431	569.030	642.659	-18.407	581.600	759.382	-158.661
298.15	419.947	636.170	636.170	0.000	575.059	794.232	-139.143
300	422.813	638.776	636.178	0.780	574.818	795.590	-138.522
350	498.186	709.671	641.605	23.823	568.806	832.875	-124.297
400	568.127	780.829	654.562	50.507	563.609	870.952	-113.732
450	631.513	851.471	672.524	80.526	559.127	909.645	-105.587
500	688.170	920.998	693.906	113.546	555.257	948.829	-99.121
600	783.083	1055.202	743.038	187.299	548.997	1028.165	-89.508
700	857.947	1181.760	796.767	269.495	544.469	1108.414	-82.709
800	917.783	1300.372	852.387	358.389	541.472	1189.187	-77.644
900	966.369	1411.372	908.397	452.677	539.805	1270.245	-73.722
1000	1006.372	1515.326	963.949	551.377	539.287	1351.443	-70.591
1100	1039.680	1612.853	1018.553	653.729	539.692	1432.658	-68.030
1200	1067.666	1704.551	1071.938	759.136	540.862	1513.778	-65.892
1300	1091.360	1790.971	1123.956	867.120	542.591	1594.791	-64.078
1400	1111.556	1872.608	1174.543	977.292	544.727	1675.659	-62.518
1500	1128.873	1949.903	1223.680	1089.335	547.182	1756.366	-61.161
1600	1143.805	2023.247	1271.381	1202.987	549.805	1836.891	-59.967
1700	1156.750	2092.988	1317.676	1318.030	552.514	1917.220	-58.908
1800	1168.027	2159.432	1362.609	1434.281	555.222	1997.468	-57.964
1900	1177.898	2222.855	1406.229	1551.588	557.895	2077.500	-57.113
2000	1186.578	2283.498	1448.588	1669.821	560.472	2157.427	-56.345
2100	1194.242	2341.581	1489.738	1788.870	562.860	2237.212	-55.646
2200	1201.039	2397.297	1529.733	1908.641	565.062	2316.889	-55.009
2300	1207.088	2450.821	1568.624	2029.053	567.073	2396.472	-54.424
2400	1212.493	2502.311	1606.462	2150.037	568.808	2475.911	-53.886
2500	1217.339	2551.907	1643.294	2271.533	570.284	2555.424	-53.392
2600	1221.699	2599.739	1679.166	2393.489	571.458	2634.739	-52.931
2700	1225.633	2645.921	1714.121	2515.859	572.336	2714.106	-52.506
2800	1229.194	2690.560	1748.201	2638.603	572.887	2793.470	-52.112
2900	1232.426	2733.751	1781.445	2761.686	573.077	2872.757	-51.743
3000	1235.369	2775.583	1813.890	2885.079	572.960	2952.075	-51.399
3100	1238.054	2816.134	1845.569	3008.752	572.441	3031.307	-51.076
3200	1240.511	2855.480	1876.517	3132.682	571.573	3110.653	-50.775
3300	1242.763	2893.688	1906.765	3256.847	570.334	3190.082	-50.494
3400	1244.834	2930.819	1936.340	3381.228	568.690	3269.444	-50.228
3500	1246.741	2966.932	1965.272	3505.808	566.647	3348.839	-49.978
3600	1248.501	3002.079	1993.587	3630.572	564.233	3428.408	-49.744
3700	1250.128	3036.309	2021.308	3755.504	561.409	3508.068	-49.524
3800	1251.636	3069.668	2048.459	3880.593	558.146	3587.738	-49.316
3900	1253.036	3102.198	2075.063	4005.828	554.491	3667.432	-49.119
4000	1254.337	3133.939	2101.139	4131.197	550.426	3747.400	-48.935
4100	1255.549	3164.927	2126.709	4256.692	545.908	3827.382	-48.760
4200	1256.679	3195.196	2151.790	4382.304	540.971	3907.469	-48.595
4300	1257.735	3224.779	2176.401	4508.025	535.599	3987.567	-48.438
4400	1258.722	3253.705	2200.557	4633.849	529.801	4067.907	-48.291
4500	1259.647	3282.002	2224.276	4759.768	523.597	4148.453	-48.153
4600	1260.515	3309.698	2247.572	4885.776	516.922	4229.155	-48.023
4700	1261.330	3336.815	2270.460	5011.869	509.794	4309.864	-47.898
4800	1262.097	3363.379	2292.954	5138.041	502.271	4390.862	-47.781
4900	1262.818	3389.410	2315.066	5264.287	494.261	4471.851	-47.670
5000	1263.498	3414.929	2336.809	5390.603	485.880	4553.239	-47.566

3.597. Dibenzo[fg,ij]naphtho[2,1,8-*uva*]pentaphene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 117726-84-8
Point Group: C₁

Length: 16.19 Å
Width: 12.31 Å
Breadth: 5.398 Å
L/B Ratio: 1.316

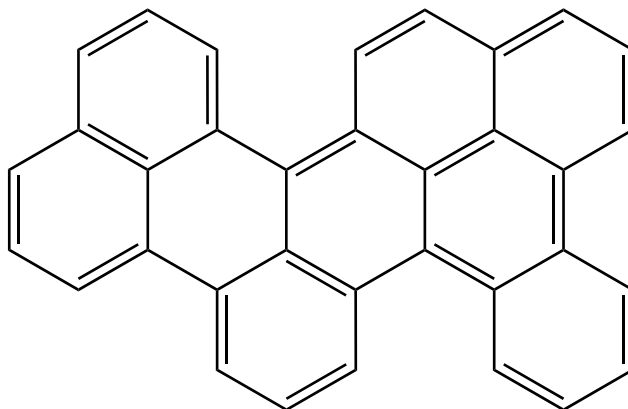
Cartesian coordinates:

C	4.5665	-3.0870	-0.5396	C	0.0474	0.2791	-0.0175	H	6.7057	-3.2600	-0.3145
C	6.0175	-1.2621	0.0808	C	-0.8355	2.6082	-0.0182	H	2.0238	-3.7617	-1.1179
C	5.8417	-2.5895	-0.2596	C	-2.1792	2.0990	-0.2765	H	0.0595	-2.3151	-0.8892
C	3.4587	-2.2503	-0.4710	C	-4.7843	1.1333	-0.5740	H	4.1165	2.8776	0.7910
C	2.1313	-2.7269	-0.7724	C	-4.5228	2.4732	-0.7562	H	6.0821	1.3582	0.7082
C	1.0569	-1.9232	-0.6440	C	-3.2241	2.9608	-0.5808	H	-1.4664	4.6619	-0.0023
C	1.1552	-0.5438	-0.2146	C	-2.4210	0.7093	-0.1637	H	0.8096	5.5517	0.4681
C	3.6175	-0.8883	-0.1145	C	-1.3324	-0.2106	0.0814	H	2.7495	3.9951	0.6127
C	2.4783	-0.0194	-0.0255	C	-1.6354	-1.4935	0.4432	H	-5.8074	0.7378	-0.6679
C	2.6756	1.3308	0.2765	C	-3.7456	0.2383	-0.2479	H	-5.3301	3.1648	-1.0183
C	3.9982	1.8113	0.5445	C	-4.0326	-1.1474	0.0450	H	-3.0242	4.0399	-0.6663
C	5.0737	0.9859	0.4952	C	-2.9792	-1.9876	0.4397	H	-0.8417	-2.2042	0.7171
C	4.9121	-0.3953	0.1541	C	-3.2520	-3.3274	0.7956	H	-2.4276	-3.9746	1.1164
C	1.5520	2.2167	0.2779	C	-4.5384	-3.8122	0.7371	H	-4.7510	-4.8506	1.0115
C	-0.6190	3.9672	0.1043	C	-5.5904	-2.9783	0.3218	H	-6.6083	-3.3784	0.2726
C	0.6678	4.4723	0.3523	C	-5.3428	-1.6676	-0.0165	H	-6.1573	-0.9993	-0.3351
C	1.7326	3.6140	0.4339	H	4.4399	-4.1398	-0.8162				
C	0.2539	1.6938	0.0954	H	7.0193	-0.8735	0.2958				

Table 3.597: Table of thermodynamic data as a function of temperature for Dibenzofg,ijnaphtho[2,1,8-*uva*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-61.049	574.235	574.235	∞
100	130.854	379.021	911.445	-53.242	603.899	659.888	-344.683
200	266.674	509.265	677.647	-33.676	588.135	722.181	-188.610
250	344.460	577.075	650.714	-18.410	580.773	756.544	-158.068
298.15	420.013	644.224	644.224	0.000	574.235	791.007	-138.578
300	422.879	646.831	644.232	0.780	573.994	792.350	-137.958
350	498.217	717.733	649.659	23.826	567.985	829.232	-123.754
400	568.096	788.892	662.618	50.510	562.788	866.905	-113.204
450	631.421	859.526	680.580	80.526	558.303	905.195	-105.070
500	688.031	929.041	701.962	113.540	554.427	943.977	-98.615
600	782.899	1063.215	751.089	187.276	548.150	1022.510	-89.016
700	857.763	1189.744	804.811	269.453	543.603	1101.960	-82.228
800	917.622	1308.333	860.421	358.330	540.589	1181.935	-77.171
900	966.238	1419.316	916.423	452.604	538.907	1262.198	-73.255
1000	1006.271	1523.257	971.965	551.292	538.377	1342.602	-70.129
1100	1039.605	1620.776	1026.562	653.635	538.774	1423.024	-67.572
1200	1067.612	1712.469	1079.939	759.036	539.938	1503.353	-65.438
1300	1091.324	1798.885	1131.951	867.015	541.662	1583.574	-63.627
1400	1111.532	1880.520	1182.531	977.184	543.795	1663.651	-62.070
1500	1128.859	1957.814	1231.664	1089.225	546.249	1743.567	-60.715
1600	1143.799	2031.157	1279.360	1202.877	548.871	1823.301	-59.523
1700	1156.749	2100.897	1325.651	1317.919	551.579	1902.839	-58.466
1800	1168.031	2167.342	1370.581	1434.171	554.287	1982.295	-57.524
1900	1177.905	2230.765	1414.197	1551.478	556.961	2061.537	-56.674
2000	1186.587	2291.409	1456.553	1669.712	559.538	2140.673	-55.907
2100	1194.253	2349.492	1497.700	1788.762	561.928	2219.666	-55.210
2200	1201.051	2405.208	1537.693	1908.534	564.131	2298.553	-54.573
2300	1207.101	2458.733	1576.582	2028.947	566.143	2377.344	-53.990
2400	1212.506	2510.223	1614.418	2149.932	567.880	2455.992	-53.452
2500	1217.353	2559.820	1651.248	2271.430	569.357	2534.714	-52.959
2600	1221.712	2607.652	1687.119	2393.387	570.532	2613.237	-52.499
2700	1225.646	2653.835	1722.073	2515.758	571.411	2691.813	-52.075
2800	1229.207	2698.474	1756.152	2638.504	571.964	2770.386	-51.681
2900	1232.439	2741.666	1789.394	2761.588	572.155	2848.881	-51.313
3000	1235.381	2783.498	1821.837	2884.982	572.039	2927.408	-50.970
3100	1238.066	2824.050	1853.516	3008.656	571.521	3005.848	-50.647
3200	1240.522	2863.397	1884.463	3132.587	570.654	3084.403	-50.347
3300	1242.775	2901.605	1914.710	3256.754	569.417	3163.040	-50.066
3400	1244.845	2938.736	1944.284	3381.136	567.773	3241.611	-49.800
3500	1246.752	2974.849	1973.216	3505.717	565.731	3320.213	-49.550
3600	1248.511	3009.996	2001.529	3630.482	563.319	3398.991	-49.317
3700	1250.139	3044.227	2029.250	3755.415	560.496	3477.859	-49.098
3800	1251.646	3077.586	2056.400	3880.505	557.233	3556.737	-48.890
3900	1253.045	3110.116	2083.003	4005.741	553.580	3635.639	-48.693
4000	1254.346	3141.857	2109.080	4131.111	549.516	3714.815	-48.510
4100	1255.558	3172.845	2134.649	4256.607	544.999	3794.005	-48.335
4200	1256.687	3203.115	2159.729	4382.220	540.063	3873.301	-48.171
4300	1257.743	3232.698	2184.339	4507.942	534.691	3952.606	-48.014
4400	1258.730	3261.624	2208.496	4633.766	528.894	4032.155	-47.867
4500	1259.655	3289.922	2232.214	4759.686	522.691	4111.909	-47.729
4600	1260.523	3317.617	2255.510	4885.695	516.016	4191.819	-47.599
4700	1261.337	3344.735	2278.397	5011.789	508.890	4271.736	-47.474
4800	1262.103	3371.299	2300.890	5137.961	501.367	4351.942	-47.358
4900	1262.825	3397.330	2323.002	5264.208	493.358	4432.139	-47.246
5000	1263.505	3422.849	2344.745	5390.525	484.978	4512.735	-47.143

3.598. Dibenzo[*j,lm*]naphtho[1,8-*ab*]perylene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 93122-98-6
Point Group: C₁

Length: 15.53 Å
Width: 11.36 Å
Breadth: 5.914 Å
L/B Ratio: 1.367

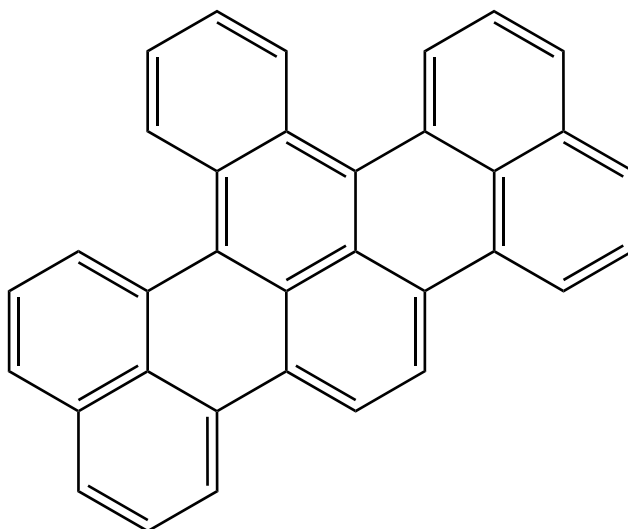
Cartesian coordinates:

C	5.1225	1.1697	0.4934	C	-1.0462	0.9541	-0.1721	H	-3.9230	-3.7435	1.8140
C	3.8656	0.6081	0.2017	C	-1.1387	-0.4535	0.0460	H	-7.0444	-0.5374	0.1891
C	2.6999	1.3865	0.3365	C	-2.4453	-1.0114	0.4017	H	-6.8519	1.7562	-0.7605
C	2.8350	2.6839	0.8701	C	-3.6230	-0.2464	0.1344	H	-4.6215	2.8203	-1.0143
C	4.0715	3.2128	1.1803	C	-3.5370	1.0953	-0.3345	H	-3.0298	3.6469	-0.9517
C	5.2300	2.4597	0.9688	C	-2.2234	1.7280	-0.4172	H	-0.7989	4.7349	-1.1247
C	1.4024	0.8126	0.0045	C	-2.5882	-2.2305	1.0346	H	1.2546	3.4526	-0.6608
C	1.2974	-0.5771	-0.1260	C	-3.8601	-2.7693	1.3177	H	1.0274	-4.4471	-0.7923
C	2.4881	-1.3808	-0.2623	C	-4.9960	-2.0936	0.9650	H	-1.0103	-3.1271	-0.4098
C	3.7653	-0.7895	-0.1749	C	-4.8960	-0.8089	0.3688	H	5.8959	-1.0964	-0.3301
C	2.3916	-2.7650	-0.5227	C	-4.6913	1.7843	-0.6486	H	5.6967	-3.5201	-0.8540
C	3.5444	-3.5264	-0.7327	C	-5.9568	1.1885	-0.4859	H	3.4567	-4.5987	-0.9410
C	4.7944	-2.9247	-0.6799	C	-6.0633	-0.0761	0.0292	H	1.9369	3.2929	1.0418
C	4.9047	-1.5704	-0.3965	C	0.2753	2.9614	-0.5787	H	4.1469	4.2235	1.5947
C	0.0172	-1.2169	-0.1342	C	-0.8602	3.6801	-0.8372	H	6.2119	2.8876	1.1946
C	-0.0250	-2.6417	-0.3721	C	-2.1193	3.0636	-0.7450	H	6.0225	0.5531	0.3451
C	1.0879	-3.3740	-0.5769	H	-5.9883	-2.5202	1.1493				
C	0.2196	1.5873	-0.2221	H	-1.7025	-2.8204	1.3075				

Table 3.598: Table of thermodynamic data as a function of temperature for Dibenzol[*j,lm*]naphtho[1,8-*ab*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-60.737	601.004	601.004	∞
100	129.747	373.525	904.527	-53.100	630.810	687.348	-359.027
200	266.008	503.222	671.275	-33.611	614.969	750.224	-195.934
250	343.778	570.881	644.393	-18.378	607.574	784.893	-163.991
298.15	419.379	637.913	637.913	0.000	601.004	819.657	-143.598
300	422.248	640.516	637.921	0.779	600.762	821.012	-142.948
350	497.687	711.329	643.341	23.796	594.724	858.212	-128.079
400	567.682	782.424	656.285	50.456	589.503	896.208	-117.030
450	631.114	853.016	674.230	80.454	585.000	934.822	-108.509
500	687.810	922.503	695.594	113.455	581.111	973.930	-101.744
600	782.790	1056.648	744.690	187.175	574.818	1053.118	-91.680
700	857.706	1183.164	798.387	269.344	570.263	1133.225	-84.561
800	917.583	1301.748	853.977	358.216	567.244	1213.859	-79.255
900	966.201	1412.726	909.963	452.487	565.559	1294.781	-75.146
1000	1006.230	1516.663	965.492	551.171	565.025	1375.844	-71.865
1100	1039.558	1614.177	1020.077	653.510	565.417	1456.926	-69.182
1200	1067.561	1705.866	1073.445	758.906	566.577	1537.914	-66.942
1300	1091.269	1792.278	1125.448	866.879	568.295	1618.796	-65.043
1400	1111.475	1873.909	1176.021	977.043	570.423	1699.534	-63.409
1500	1128.801	1951.199	1225.146	1089.078	572.870	1780.111	-61.988
1600	1143.742	2024.539	1272.836	1202.724	575.487	1860.507	-60.738
1700	1156.693	2094.275	1319.122	1317.761	578.190	1940.707	-59.629
1800	1167.976	2160.717	1364.046	1434.007	580.892	2020.826	-58.642
1900	1177.852	2224.136	1407.658	1551.309	583.560	2100.730	-57.752
2000	1186.536	2284.778	1450.009	1669.537	586.132	2180.529	-56.948
2100	1194.204	2342.858	1491.152	1788.582	588.517	2260.186	-56.218
2200	1201.004	2398.573	1531.141	1908.349	590.715	2339.736	-55.551
2300	1207.056	2452.096	1570.027	2028.758	592.723	2419.191	-54.940
2400	1212.464	2503.584	1607.859	2149.739	594.455	2498.503	-54.377
2500	1217.312	2553.179	1644.686	2271.232	595.928	2577.888	-53.861
2600	1221.673	2601.009	1680.553	2393.185	597.099	2657.076	-53.380
2700	1225.609	2647.191	1715.505	2515.553	597.975	2736.316	-52.936
2800	1229.172	2691.829	1749.581	2638.295	598.524	2815.553	-52.524
2900	1232.406	2735.019	1782.821	2761.376	598.711	2894.713	-52.138
3000	1235.349	2776.850	1815.261	2884.766	598.592	2973.905	-51.779
3100	1238.036	2817.401	1846.938	3008.437	598.071	3053.010	-51.442
3200	1240.493	2856.747	1877.883	3132.366	597.202	3132.229	-51.127
3300	1242.747	2894.954	1908.127	3256.529	595.961	3211.532	-50.833
3400	1244.819	2932.085	1937.700	3380.909	594.315	3290.767	-50.555
3500	1246.726	2968.197	1966.629	3505.488	592.271	3370.035	-50.294
3600	1248.487	3003.343	1994.941	3630.249	589.855	3449.478	-50.050
3700	1250.116	3037.573	2022.659	3755.181	587.031	3529.011	-49.820
3800	1251.624	3070.932	2049.808	3880.269	583.766	3608.555	-49.602
3900	1253.024	3103.462	2076.410	4005.502	580.110	3688.123	-49.396
4000	1254.326	3135.202	2102.485	4130.870	576.044	3767.964	-49.204
4100	1255.538	3166.190	2128.052	4256.364	571.525	3847.820	-49.021
4200	1256.669	3196.459	2153.131	4381.975	566.587	3927.781	-48.848
4300	1257.725	3226.041	2177.740	4507.695	561.213	4007.752	-48.684
4400	1258.713	3254.967	2201.895	4633.518	555.415	4087.967	-48.529
4500	1259.639	3283.265	2225.612	4759.436	549.210	4168.386	-48.384
4600	1260.507	3310.960	2248.907	4885.444	542.534	4248.962	-48.247
4700	1261.322	3338.077	2271.793	5011.536	535.406	4329.545	-48.117
4800	1262.089	3364.641	2294.285	5137.707	527.882	4410.416	-47.994
4900	1262.811	3390.671	2316.396	5263.952	519.871	4491.279	-47.877
5000	1263.491	3416.191	2338.137	5390.267	511.489	4572.541	-47.768

3.599. Tetrabenzo[*de,h,kl,rst*]pentaphene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 188-13-6
Point Group: C₂

Length: 16.02 Å
Width: 11.62 Å
Breadth: 5.489 Å
L/B Ratio: 1.379

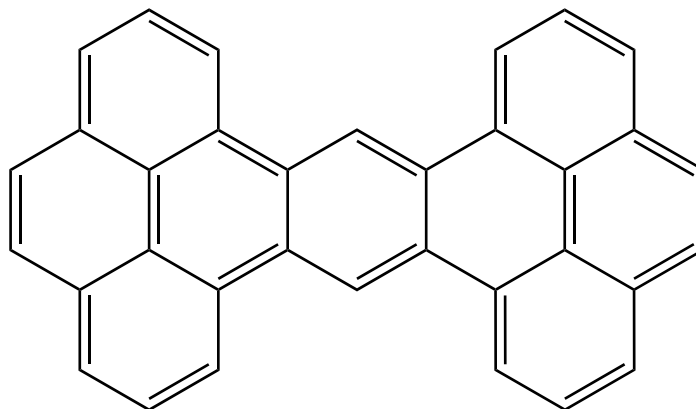
Cartesian coordinates:

C	5.0457	-1.6758	-0.8506	C	-0.6946	-4.4363	-0.1496	H	3.1561	-2.6668	-1.1292
C	5.7138	-0.5667	-0.4095	C	0.6935	-4.4365	0.1478	H	6.7385	1.7647	0.4555
C	3.6391	-1.7449	-0.7778	C	1.3640	-3.2567	0.2176	H	5.4268	3.7925	1.0619
C	4.9782	0.5626	0.0354	C	-0.7118	0.4329	-0.0063	H	2.9443	3.7796	0.8538
C	5.6431	1.7542	0.4269	C	-1.3958	1.6908	-0.1329	H	1.2333	3.8273	0.2106
C	4.9210	2.8722	0.7521	C	-1.4325	-0.7790	0.0661	H	-1.2331	3.8274	-0.2120
C	3.5157	2.8582	0.6642	C	-2.8865	-0.7081	0.2609	H	-2.4408	-3.2644	-0.4407
C	2.8866	-0.7083	-0.2603	C	-5.7136	-0.5665	0.4107	H	-1.2086	-5.3890	-0.3115
C	3.5679	0.5113	0.0484	C	-5.0453	-1.6754	0.8523	H	1.2073	-5.3896	0.3088
C	2.8424	1.7060	0.3106	C	-3.6387	-1.7445	0.7792	H	2.4402	-3.2658	0.4390
C	1.3959	1.6908	0.1324	C	-3.5678	0.5114	-0.0481	H	-6.8083	-0.5228	0.4199
C	0.6975	2.8728	0.0931	C	-2.8423	1.7060	-0.3109	H	-5.5956	-2.5333	1.2531
C	-0.6973	2.8728	-0.0940	C	-3.5157	2.8580	-0.6648	H	-3.1552	-2.6658	1.1313
C	0.7119	0.4328	0.0062	C	-4.9210	2.8720	-0.7524	H	-2.9443	3.7794	-0.8548
C	1.4326	-0.7792	-0.0659	C	-5.6431	1.7541	-0.4266	H	-5.4269	3.7922	-1.0623
C	0.7131	-1.9919	0.0251	C	-4.9781	0.5627	-0.0348	H	-6.7385	1.7647	-0.4551
C	-0.7133	-1.9918	-0.0252	H	5.5961	-2.5340	-1.2508				
C	-1.3647	-3.2562	-0.2187	H	6.8085	-0.5230	-0.4185				

Table 3.599: Table of thermodynamic data as a function of temperature for Tetra-benzo[de,h,kl,rst]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-61.076	647.790	647.790	∞
100	130.853	369.679	903.352	-53.367	677.329	734.252	-383.526
200	267.329	500.174	668.981	-33.762	661.605	797.469	-208.273
250	345.329	568.152	641.980	-18.457	654.281	832.282	-173.892
298.15	421.101	635.473	635.473	0.000	647.790	867.171	-151.922
300	423.975	638.087	635.481	0.782	647.551	868.530	-151.221
350	499.511	709.174	640.923	23.888	641.602	905.845	-135.187
400	569.531	780.515	653.915	50.640	636.473	943.942	-123.264
450	632.935	851.324	671.923	80.730	632.062	982.646	-114.060
500	689.566	920.999	693.359	113.820	628.262	1021.833	-106.748
600	784.360	1055.449	742.603	187.708	622.137	1101.156	-95.862
700	859.073	1182.192	796.444	270.024	617.729	1181.372	-88.153
800	918.759	1300.945	852.167	359.023	614.837	1262.094	-82.405
900	967.213	1412.052	908.272	453.402	613.260	1343.089	-77.949
1000	1007.102	1516.089	963.908	552.181	612.821	1424.214	-74.392
1100	1040.314	1613.680	1018.589	654.601	613.294	1505.350	-71.482
1200	1068.219	1705.430	1072.041	760.067	614.524	1586.385	-69.052
1300	1091.846	1791.892	1124.121	868.102	616.304	1667.307	-66.992
1400	1111.984	1873.563	1174.763	978.320	618.486	1748.082	-65.220
1500	1129.254	1950.886	1223.950	1090.404	620.982	1828.692	-63.679
1600	1144.145	2024.253	1271.696	1204.092	623.641	1909.117	-62.325
1700	1157.055	2094.013	1318.033	1319.167	626.382	1989.345	-61.124
1800	1168.302	2160.474	1363.003	1435.447	629.118	2069.489	-60.054
1900	1178.147	2223.911	1406.658	1552.781	631.818	2149.417	-59.090
2000	1186.804	2284.566	1449.048	1671.037	634.418	2229.237	-58.221
2100	1194.449	2342.660	1490.227	1790.108	636.829	2308.915	-57.430
2200	1201.228	2398.385	1530.249	1909.898	639.050	2388.484	-56.709
2300	1207.263	2451.917	1569.166	2030.329	641.080	2467.957	-56.048
2400	1212.654	2503.414	1607.027	2151.329	642.831	2547.286	-55.439
2500	1217.488	2553.017	1643.880	2272.841	644.323	2626.688	-54.881
2600	1221.837	2600.854	1679.773	2394.811	645.511	2705.892	-54.361
2700	1225.761	2647.041	1714.747	2517.194	646.402	2785.147	-53.881
2800	1229.314	2691.684	1748.845	2639.951	646.966	2864.399	-53.435
2900	1232.538	2734.880	1782.105	2763.046	647.167	2943.573	-53.018
3000	1235.474	2776.715	1814.565	2886.449	647.061	3022.779	-52.630
3100	1238.152	2817.270	1846.260	3010.132	646.552	3101.897	-52.266
3200	1240.603	2856.619	1877.222	3134.072	645.694	3181.130	-51.926
3300	1242.850	2894.830	1907.482	3258.246	644.464	3260.445	-51.607
3400	1244.916	2931.964	1937.071	3382.636	642.828	3339.692	-51.307
3500	1246.818	2968.078	1966.014	3507.224	640.793	3418.973	-51.024
3600	1248.574	3003.227	1994.340	3631.995	638.387	3498.427	-50.760
3700	1250.198	3037.459	2022.072	3756.934	635.570	3577.972	-50.511
3800	1251.703	3070.820	2049.233	3882.030	632.313	3657.527	-50.275
3900	1253.099	3103.352	2075.847	4007.271	628.665	3737.105	-50.052
4000	1254.397	3135.094	2101.933	4132.647	624.607	3816.957	-49.843
4100	1255.606	3166.084	2127.511	4258.148	620.095	3896.824	-49.645
4200	1256.733	3196.354	2152.601	4383.765	615.163	3976.795	-49.458
4300	1257.787	3225.938	2177.219	4509.492	609.796	4056.777	-49.279
4400	1258.772	3254.866	2201.384	4635.320	604.003	4137.002	-49.111
4500	1259.695	3283.164	2225.110	4761.244	597.804	4217.431	-48.954
4600	1260.561	3310.861	2248.413	4887.257	591.133	4298.017	-48.805
4700	1261.374	3337.979	2271.308	5013.354	584.010	4378.610	-48.662
4800	1262.138	3364.544	2293.808	5139.530	576.491	4459.491	-48.528
4900	1262.858	3390.576	2315.926	5265.781	568.486	4540.364	-48.400
5000	1263.537	3416.096	2337.675	5392.101	560.109	4621.636	-48.281

3.600. Tetrabenzo[*de,jk,op,uv*]pentacene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 109587-17-9
Point Group: D_{2h}

Length: 16.59 Å
Width: 11.63 Å
Breadth: 3.885 Å
L/B Ratio: 1.427

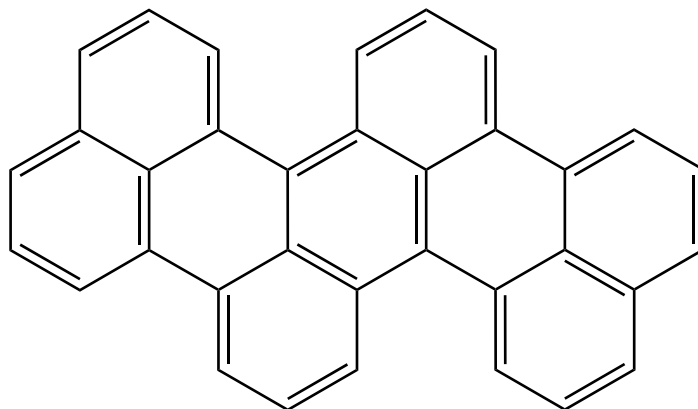
Cartesian coordinates:

C	-4.9200	2.8262	0.0000	C	1.2200	0.7039	0.0000	H	-3.7236	4.6142	0.0000
C	-2.5089	2.8327	0.0000	C	1.2183	-0.7068	0.0000	H	-7.0947	1.2496	0.0000
C	-3.7232	3.5192	0.0000	C	2.4808	1.4349	0.0000	H	-7.0976	-1.2329	0.0000
C	-4.9209	1.4221	0.0000	C	4.9266	2.8147	0.0000	H	-5.8810	-3.3532	0.0000
C	-6.1560	0.6837	0.0000	C	3.7315	3.5104	0.0000	H	-3.7343	-4.6055	0.0000
C	-6.1576	-0.6692	0.0000	C	2.5156	2.8268	0.0000	H	-1.5664	-3.3847	0.0000
C	-4.9242	-1.4106	0.0000	C	2.4774	-1.4407	0.0000	H	-0.0030	-2.4920	0.0000
C	-4.9266	-2.8147	0.0000	C	2.5089	-2.8327	0.0000	H	0.0029	2.4921	0.0000
C	-3.7314	-3.5104	0.0000	C	3.7231	-3.5192	0.0000	H	5.8811	3.3531	0.0000
C	-2.5155	-2.8268	0.0000	C	4.9199	-2.8263	0.0000	H	3.7344	4.6055	0.0000
C	-3.6967	0.7230	0.0000	C	3.6984	0.7143	0.0000	H	1.5665	3.3848	0.0000
C	-3.6984	-0.7143	0.0000	C	3.6967	-0.7230	0.0000	H	1.5584	-3.3884	0.0000
C	-2.4808	-1.4349	0.0000	C	4.9209	-1.4222	0.0000	H	3.7234	-4.6143	0.0000
C	-2.4774	1.4407	0.0000	C	6.1560	-0.6838	0.0000	H	5.8731	-3.3670	0.0000
C	-1.2184	0.7068	0.0000	C	6.1576	0.6692	0.0000	H	7.0947	-1.2496	0.0000
C	-1.2200	-0.7039	0.0000	C	4.9243	1.4106	0.0000	H	7.0977	1.2328	0.0000
C	-0.0016	-1.3847	0.0000	H	-5.8731	3.3670	0.0000				
C	0.0016	1.3847	0.0000	H	-1.5585	3.3884	0.0000				

Table 3.600: Table of thermodynamic data as a function of temperature for Tetra-benzo[*de,jk,op,uv*]pentacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-60.890	517.375	517.375	∞
100	130.855	370.624	900.867	-53.024	547.257	604.086	-315.536
200	265.468	500.385	668.059	-33.535	531.417	667.239	-174.261
250	343.006	567.898	641.238	-18.335	523.989	702.053	-146.683
298.15	418.364	634.773	634.773	0.000	517.375	736.965	-129.111
300	421.223	637.370	634.781	0.777	517.131	738.325	-128.551
350	496.419	708.006	640.188	23.736	511.036	775.687	-115.763
400	566.224	778.919	653.099	50.328	505.746	813.853	-106.276
450	629.537	849.332	670.998	80.250	501.167	852.647	-98.971
500	686.180	918.649	692.309	113.170	497.198	891.944	-93.179
600	781.198	1052.498	741.284	186.728	490.743	971.533	-84.578
700	856.256	1178.779	794.857	268.745	486.035	1052.067	-78.505
800	916.307	1297.180	850.329	357.481	482.880	1133.149	-73.986
900	965.097	1408.018	906.204	451.632	481.076	1214.535	-70.488
1000	1005.281	1511.847	961.633	550.214	480.440	1296.074	-67.699
1100	1038.742	1609.277	1016.127	652.465	480.743	1377.642	-65.417
1200	1066.857	1700.900	1069.412	757.785	481.827	1459.124	-63.513
1300	1090.658	1787.259	1121.342	865.693	483.480	1540.506	-61.897
1400	1110.943	1868.848	1171.848	975.799	485.551	1621.748	-60.507
1500	1128.335	1946.103	1220.913	1087.785	487.948	1702.833	-59.297
1600	1143.330	2019.415	1268.548	1201.386	490.521	1783.739	-58.232
1700	1156.328	2089.128	1314.784	1316.384	493.185	1864.453	-57.286
1800	1167.650	2155.549	1359.663	1432.596	495.853	1945.088	-56.444
1900	1177.559	2218.952	1403.233	1549.867	498.490	2025.510	-55.684
2000	1186.272	2279.579	1445.545	1668.068	501.035	2105.828	-54.997
2100	1193.965	2337.648	1486.654	1787.088	503.394	2186.005	-54.373
2200	1200.786	2393.352	1526.610	1906.832	505.570	2266.076	-53.802
2300	1206.858	2446.865	1565.465	2027.220	507.557	2346.054	-53.279
2400	1212.282	2498.345	1603.270	2148.182	509.270	2425.889	-52.797
2500	1217.145	2547.934	1640.070	2269.658	510.725	2505.799	-52.355
2600	1221.519	2595.758	1675.913	2391.595	511.880	2585.511	-51.942
2700	1225.466	2641.933	1710.842	2513.947	512.741	2665.277	-51.562
2800	1229.039	2686.566	1744.896	2636.676	513.276	2745.040	-51.208
2900	1232.282	2729.752	1778.116	2759.744	513.451	2824.726	-50.878
3000	1235.234	2771.579	1810.538	2883.122	513.320	2904.445	-50.570
3100	1237.928	2812.127	1842.197	3006.782	512.788	2984.077	-50.280
3200	1240.393	2851.469	1873.125	3130.700	511.908	3063.825	-50.011
3300	1242.652	2889.673	1903.354	3254.854	510.658	3143.655	-49.759
3400	1244.729	2926.801	1932.912	3379.225	509.002	3223.419	-49.521
3500	1246.642	2962.911	1961.827	3503.795	506.949	3303.215	-49.297
3600	1248.408	2998.055	1990.125	3628.548	504.526	3383.187	-49.088
3700	1250.041	3032.282	2017.831	3753.472	501.693	3463.249	-48.891
3800	1251.553	3065.639	2044.968	3878.552	498.421	3543.322	-48.705
3900	1252.957	3098.167	2071.557	4003.779	494.758	3623.419	-48.529
4000	1254.262	3129.906	2097.621	4129.140	490.686	3703.790	-48.366
4100	1255.477	3160.892	2123.178	4254.628	486.161	3784.175	-48.210
4200	1256.611	3191.160	2148.247	4380.233	481.217	3864.666	-48.063
4300	1257.670	3220.741	2172.846	4505.948	475.837	3945.167	-47.923
4400	1258.660	3249.666	2196.992	4631.765	470.033	4025.912	-47.793
4500	1259.588	3277.962	2220.700	4757.678	463.823	4106.861	-47.670
4600	1260.459	3305.656	2243.986	4883.681	457.142	4187.968	-47.555
4700	1261.276	3332.772	2266.864	5009.768	450.009	4269.081	-47.445
4800	1262.045	3359.335	2289.349	5135.934	442.481	4350.483	-47.342
4900	1262.768	3385.365	2311.451	5262.175	434.466	4431.877	-47.243
5000	1263.450	3410.883	2333.186	5388.486	426.080	4513.670	-47.153

3.601. Tetrabenzo[*de,hi,op,st*]pentacene



Other names: 1,9,5,10-Di(peri-naphthylene)anthracene

Formula: C₃₄H₁₈

Mass: 426.507 g/mol

CAS Number: 191-79-7

Point Group: C₂

Length: 16.65 Å

Width: 11.30 Å

Breadth: 5.795 Å

L/B Ratio: 1.473

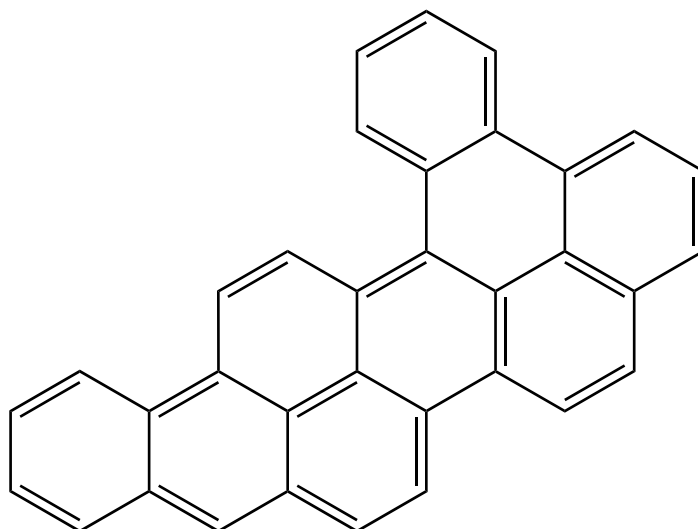
Cartesian coordinates:

C	5.2690	-1.9472	-0.8859	C	-2.0446	-3.0520	0.6329	H	4.3112	-3.6934	-1.6783
C	2.8762	-2.2518	-0.9440	C	-0.7390	-3.5889	0.6870	H	7.2059	-0.2315	-0.1609
C	4.1815	-2.7102	-1.2136	C	0.3397	-2.7884	0.4624	H	6.8566	2.0745	0.7102
C	5.0813	-0.6542	-0.3315	C	-1.1186	-0.8428	0.1723	H	4.5574	2.9926	0.9287
C	6.1955	0.1674	-0.0166	C	-1.3098	0.5437	-0.0059	H	2.9098	3.7095	0.8107
C	6.0026	1.4383	0.4558	C	-2.2420	-1.7184	0.3740	H	0.6104	4.6520	0.9180
C	4.6990	1.9517	0.5996	C	-3.5952	-1.1743	0.3127	H	-1.3508	3.2161	0.5115
C	3.7724	-0.1730	-0.1134	C	-6.1957	-0.1683	-0.0186	H	-2.9098	-3.7088	0.8116
C	3.5952	1.1746	0.3107	C	-6.0028	-1.4392	0.4537	H	-0.6101	-4.6517	0.9167
C	2.6492	-1.0247	-0.3513	C	-4.6993	-1.9520	0.5993	H	1.3505	-3.2167	0.5078
C	2.2419	1.7190	0.3714	C	-3.7726	0.1732	-0.1114	H	-7.2061	0.2299	-0.1648
C	2.0449	3.0526	0.6308	C	-2.6495	1.0253	-0.3488	H	-6.8569	-2.0762	0.7060
C	0.7393	3.5893	0.6873	C	-2.8760	2.2517	-0.9431	H	-4.5570	-2.9929	0.9283
C	-0.3396	2.7888	0.4641	C	-4.1811	2.7094	-1.2147	H	-2.0329	2.9092	-1.1959
C	1.1186	0.8433	0.1701	C	-5.2687	1.9466	-0.8866	H	-4.3107	3.6919	-1.6808
C	-0.1955	1.3932	0.1895	C	-5.0813	0.6539	-0.3315	H	-6.2875	2.3099	-1.0624
C	1.3096	-0.5432	-0.0083	H	6.2878	-2.3111	-1.0594				
C	0.1955	-1.3927	0.1892	H	2.0335	-2.9103	-1.1958				

Table 3.601: Table of thermodynamic data as a function of temperature for Tetra-benzo[*de,hi,op,st*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	–61.046	634.924	634.924	∞
100	130.573	371.776	904.750	–53.297	664.532	721.246	–376.732
200	267.018	502.088	670.677	–33.718	648.782	784.263	–204.824
250	344.880	569.982	643.712	–18.432	641.439	818.983	–171.114
298.15	420.534	637.213	637.213	0.000	634.924	853.786	–149.577
300	423.404	639.823	637.221	0.781	634.683	855.141	–148.890
350	498.863	710.816	642.656	23.856	628.704	892.372	–133.176
400	568.847	782.068	655.631	50.575	623.542	930.389	–121.494
450	632.244	852.796	673.617	80.631	619.096	969.017	–112.478
500	688.892	922.399	695.026	113.687	615.262	1008.133	–105.317
600	783.751	1056.731	744.216	187.509	609.072	1087.322	–94.658
700	858.542	1183.386	798.003	269.768	604.607	1167.414	–87.112
800	918.304	1302.073	853.675	358.718	601.666	1248.020	–81.486
900	966.825	1413.131	909.735	453.056	600.047	1328.905	–77.126
1000	1006.770	1517.129	965.331	551.798	599.572	1409.925	–73.645
1100	1040.029	1614.692	1019.976	654.188	600.014	1490.957	–70.798
1200	1067.973	1706.418	1073.396	759.627	601.218	1571.892	–68.421
1300	1091.632	1792.862	1125.447	867.640	602.975	1652.718	–66.406
1400	1111.797	1874.518	1176.063	977.837	605.137	1733.396	–64.672
1500	1129.089	1951.829	1225.226	1089.903	607.615	1813.911	–63.165
1600	1143.999	2025.186	1272.951	1203.576	610.258	1894.242	–61.839
1700	1156.925	2094.938	1319.269	1318.637	612.986	1974.377	–60.664
1800	1168.185	2161.392	1364.222	1434.905	615.710	2054.429	–59.617
1900	1178.042	2224.822	1407.860	1552.227	618.398	2134.266	–58.674
2000	1186.709	2285.473	1450.236	1670.474	620.989	2213.995	–57.822
2100	1194.363	2343.561	1491.402	1789.535	623.390	2293.582	–57.049
2200	1201.149	2399.283	1531.411	1909.318	625.603	2373.061	–56.342
2300	1207.190	2452.812	1570.316	2029.741	627.625	2452.445	–55.696
2400	1212.588	2504.306	1608.166	2150.734	629.370	2531.685	–55.100
2500	1217.427	2553.906	1645.010	2272.239	630.855	2610.998	–54.553
2600	1221.780	2601.740	1680.893	2394.204	632.037	2690.113	–54.044
2700	1225.709	2647.926	1715.859	2516.581	632.923	2769.280	–53.574
2800	1229.265	2692.567	1749.948	2639.333	633.482	2848.443	–53.137
2900	1232.493	2735.761	1783.201	2762.423	633.678	2927.529	–52.729
3000	1235.431	2777.595	1815.654	2885.822	633.567	3006.647	–52.349
3100	1238.112	2818.149	1847.342	3009.501	633.055	3085.677	–51.992
3200	1240.565	2857.496	1878.297	3133.437	632.192	3164.822	–51.659
3300	1242.815	2895.706	1908.552	3257.607	630.959	3244.049	–51.348
3400	1244.883	2932.838	1938.134	3381.994	629.319	3323.209	–51.054
3500	1246.787	2968.952	1967.073	3506.578	627.281	3402.402	–50.777
3600	1248.545	3004.100	1995.393	3631.346	624.872	3481.769	–50.518
3700	1250.170	3038.332	2023.120	3756.283	622.053	3561.227	–50.274
3800	1251.676	3071.692	2050.277	3881.376	618.793	3640.694	–50.044
3900	1253.073	3104.223	2076.886	4006.614	615.142	3720.186	–49.825
4000	1254.373	3135.965	2102.968	4131.988	611.081	3799.951	–49.621
4100	1255.583	3166.953	2128.542	4257.486	606.567	3879.731	–49.427
4200	1256.712	3197.224	2153.628	4383.101	601.633	3959.615	–49.244
4300	1257.766	3226.807	2178.243	4508.826	596.264	4039.510	–49.069
4400	1258.752	3255.734	2202.404	4634.652	590.469	4119.648	–48.905
4500	1259.676	3284.032	2226.127	4760.574	584.268	4199.990	–48.751
4600	1260.542	3311.728	2249.427	4886.586	577.595	4280.489	–48.605
4700	1261.356	3338.846	2272.318	5012.681	570.471	4360.996	–48.466
4800	1262.122	3365.410	2294.815	5138.855	562.950	4441.790	–48.336
4900	1262.842	3391.442	2316.931	5265.104	554.942	4522.576	–48.210
5000	1263.521	3416.962	2338.677	5391.422	546.564	4603.761	–48.094

3.602. Dibenzo[*a,rst*]naphtho[8,1,2-*cde*]pentaphene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 191-46-8
Point Group: C₁

Length: 17.96 Å
Width: 11.60 Å
Breadth: 5.098 Å
L/B Ratio: 1.548

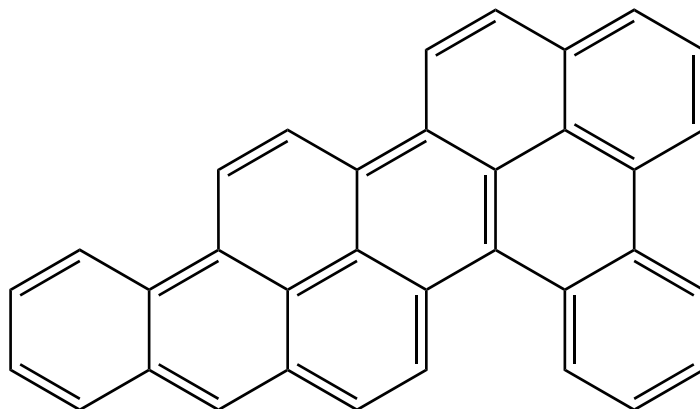
Cartesian coordinates:

C	1.5601	2.9955	-0.6797	C	-3.0378	-1.8219	-0.2865	H	-7.0871	-1.5363	-0.2118
C	2.0928	1.7732	-0.2291	C	-2.3057	-3.0447	-0.5165	H	-4.5958	2.6960	0.6797
C	3.4808	1.7153	0.0058	C	-0.9580	-3.0580	-0.4949	H	-4.9765	-2.7370	-0.4566
C	4.2559	2.8852	-0.0720	C	-2.9950	0.5734	0.1984	H	-2.8781	-3.9613	-0.7008
C	3.6928	4.0874	-0.4511	C	-4.4240	0.5843	0.2194	H	-0.4002	-3.9937	-0.6521
C	2.3389	4.1322	-0.7870	C	-5.1279	-0.6129	-0.0270	H	-0.3380	2.6854	0.6061
C	4.1292	0.4368	0.2447	C	-4.4154	-1.8117	-0.2756	H	-2.7958	2.6722	0.7223
C	3.3670	-0.7447	0.1118	C	-6.5502	-0.6011	-0.0164	H	1.3338	-4.0601	-0.3272
C	1.9381	-0.6777	-0.0667	C	-7.2315	0.5586	0.2343	H	3.7868	-4.1579	0.0331
C	1.2741	0.5709	-0.0812	C	-6.5277	1.7586	0.4880	H	5.8865	-3.0297	0.5431
C	1.2118	-1.8879	-0.1777	C	-5.1595	1.7715	0.4815	H	7.1871	-0.9355	0.8774
C	1.9216	-3.1415	-0.1785	C	-2.2389	1.7597	0.4582	H	6.0746	1.2757	0.6469
C	3.2569	-3.1987	0.0133	C	-0.8858	1.7587	0.3863	H	5.3303	2.8235	0.1603
C	4.0183	-1.9935	0.2001	C	5.4915	0.3494	0.5309	H	4.3046	4.9932	-0.5084
C	-0.1365	0.5801	0.0501	C	6.1170	-0.8884	0.6505	H	1.8943	5.0697	-1.1369
C	-0.8666	-0.6285	-0.0959	C	5.3925	-2.0542	0.4706	H	0.4993	3.0567	-0.9586
C	-0.1908	-1.8561	-0.2678	H	-7.0920	2.6750	0.6896				
C	-2.3039	-0.6144	-0.0610	H	-8.3263	0.5717	0.2426				

Table 3.602: Table of thermodynamic data as a function of temperature for Dibenzo[*a,rst*]naphtho[8,1,2-*cde*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-61.229	564.606	564.606	∞
100	131.548	380.967	914.541	-53.357	594.155	649.949	-339.492
200	267.265	511.655	680.294	-33.728	578.455	712.023	-185.957
250	344.983	579.590	653.323	-18.433	571.121	746.263	-155.920
298.15	420.464	646.825	646.825	0.000	564.606	780.603	-136.756
300	423.326	649.435	646.833	0.781	564.366	781.941	-136.145
350	498.590	720.401	652.265	23.847	558.378	818.691	-122.180
400	568.403	791.604	665.234	50.548	553.197	856.230	-111.810
450	631.672	862.272	683.210	80.578	548.726	894.383	-103.815
500	688.235	931.810	704.604	113.603	544.861	933.027	-97.471
600	783.030	1066.015	753.755	187.356	538.601	1011.281	-88.038
700	857.844	1192.560	807.498	269.544	534.065	1090.450	-81.369
800	917.667	1311.158	863.124	358.427	531.057	1170.144	-76.401
900	966.259	1422.144	919.140	452.704	529.378	1250.124	-72.554
1000	1006.274	1526.087	974.694	551.393	528.850	1330.245	-69.483
1100	1039.596	1623.605	1029.299	653.736	529.246	1410.384	-66.972
1200	1067.595	1715.296	1082.684	759.135	530.409	1490.430	-64.875
1300	1091.301	1801.711	1134.702	867.112	532.131	1570.369	-63.097
1400	1111.506	1883.344	1185.288	977.279	534.261	1650.163	-61.567
1500	1128.831	1960.636	1234.425	1089.318	536.712	1729.797	-60.236
1600	1143.771	2033.978	1282.124	1202.966	539.331	1809.248	-59.065
1700	1156.721	2103.716	1328.419	1318.006	542.037	1888.504	-58.025
1800	1168.002	2170.159	1373.351	1434.255	544.742	1967.679	-57.099
1900	1177.877	2233.580	1416.970	1551.559	547.413	2046.639	-56.265
2000	1186.560	2294.223	1459.328	1669.790	549.988	2125.494	-55.511
2100	1194.228	2352.305	1500.477	1788.837	552.375	2204.206	-54.825
2200	1201.026	2408.020	1540.472	1908.607	554.575	2282.811	-54.200
2300	1207.077	2461.544	1579.363	2029.018	556.585	2361.321	-53.626
2400	1212.484	2513.033	1617.200	2150.001	558.319	2439.688	-53.097
2500	1217.331	2562.629	1654.031	2271.496	559.794	2518.129	-52.612
2600	1221.692	2610.460	1689.902	2393.451	560.967	2596.371	-52.161
2700	1225.626	2656.642	1724.857	2515.820	561.844	2674.666	-51.743
2800	1229.188	2701.281	1758.937	2638.564	562.395	2752.958	-51.356
2900	1232.421	2744.472	1792.180	2761.647	562.584	2831.173	-50.994
3000	1235.364	2786.304	1824.624	2885.038	562.467	2909.419	-50.656
3100	1238.050	2826.855	1856.303	3008.711	561.947	2987.579	-50.339
3200	1240.507	2866.201	1887.251	3132.641	561.079	3065.853	-50.044
3300	1242.760	2904.409	1917.498	3256.806	559.840	3144.210	-49.768
3400	1244.831	2941.540	1947.073	3381.187	558.195	3222.500	-49.507
3500	1246.738	2977.652	1976.005	3505.766	556.152	3300.823	-49.261
3600	1248.499	3012.799	2004.319	3630.529	553.738	3379.320	-49.032
3700	1250.126	3047.029	2032.039	3755.462	550.914	3457.907	-48.816
3800	1251.635	3080.388	2059.191	3880.551	547.650	3536.506	-48.612
3900	1253.034	3112.918	2085.794	4005.785	543.995	3615.128	-48.418
4000	1254.336	3144.659	2111.870	4131.154	539.931	3694.023	-48.238
4100	1255.547	3175.647	2137.440	4256.649	535.413	3772.933	-48.067
4200	1256.678	3205.916	2162.521	4382.261	530.475	3851.948	-47.905
4300	1257.734	3235.499	2187.131	4507.982	525.103	3930.974	-47.751
4400	1258.721	3264.425	2211.287	4633.805	519.305	4010.243	-47.607
4500	1259.646	3292.723	2235.006	4759.724	513.101	4089.716	-47.471
4600	1260.514	3320.418	2258.302	4885.733	506.425	4169.346	-47.343
4700	1261.329	3347.536	2281.190	5011.825	499.298	4248.984	-47.221
4800	1262.096	3374.099	2303.683	5137.997	491.774	4328.909	-47.107
4900	1262.817	3400.130	2325.795	5264.243	483.764	4408.827	-46.998
5000	1263.498	3425.649	2347.537	5390.559	475.384	4489.143	-46.897

3.603. Benzo[*rst*]phenanthro[1,10,9-*cde*]pentaphene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 190-93-2
Point Group: C₁

Length: 17.93 Å
Width: 11.60 Å
Breadth: 5.081 Å
L/B Ratio: 1.545

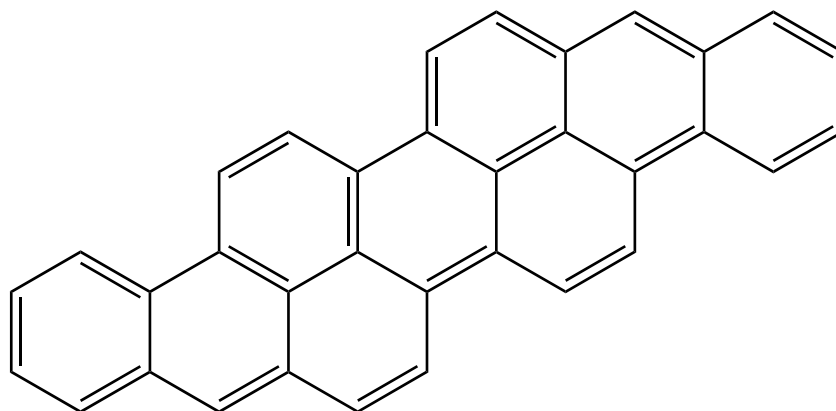
Cartesian coordinates:

C	-4.8158	2.3012	-0.1134	C	3.2583	-0.8223	-0.1171	H	6.7401	2.1701	0.4472
C	-3.8253	1.3111	-0.0158	C	4.6557	-0.5035	-0.0756	H	5.3270	-2.5175	-0.5149
C	-2.4699	1.6510	-0.1957	C	5.0563	0.8198	0.1976	H	4.4059	2.8421	0.6634
C	-2.1775	2.9619	-0.6102	C	4.0772	1.8200	0.4377	H	2.0667	3.5096	0.9661
C	-3.1654	3.9224	-0.7366	C	6.4401	1.1376	0.2345	H	-0.3226	3.0077	0.7721
C	-4.4927	3.6003	-0.4573	C	7.3805	0.1679	0.0079	H	1.1502	-3.4866	-0.5750
C	-1.4271	0.6361	-0.0295	C	6.9819	-1.1593	-0.2640	H	3.5802	-2.9282	-0.5468
C	-1.8345	-0.7328	-0.0646	C	5.6525	-1.4872	-0.3044	H	-6.2974	0.3491	0.5256
C	-3.2247	-1.0822	0.0630	C	2.8156	-2.1551	-0.3744	H	-6.9542	-2.0428	0.6871
C	-4.2138	-0.0772	0.1843	C	1.4914	-2.4557	-0.3957	H	-5.2535	-3.8303	0.3727
C	-0.8858	-1.7639	-0.1582	C	-3.6156	-2.4364	0.1116	H	-2.9516	-4.5063	-0.0652
C	0.5001	-1.4472	-0.1862	C	-4.9631	-2.7744	0.3311	H	-0.5528	-3.9093	-0.3262
C	0.9033	-0.1184	0.0313	C	-5.9073	-1.7821	0.4998	H	-1.1408	3.2415	-0.8427
C	-0.0695	0.9197	0.1640	C	-5.5358	-0.4384	0.4193	H	-2.9049	4.9368	-1.0561
C	2.3054	0.1806	0.0996	C	-1.3203	-3.1312	-0.1952	H	-5.2724	4.3650	-0.5302
C	2.7387	1.5135	0.3922	C	-2.6261	-3.4599	-0.0567	H	-5.8641	2.0215	0.0736
C	1.7303	2.5123	0.6589	H	7.7478	-1.9212	-0.4417				
C	0.4189	2.2282	0.5475	H	8.4479	0.4097	0.0353				

Table 3.603: Table of thermodynamic data as a function of temperature for Benzo[*rst*]phenanthro[1,10,9-*cde*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-61.097	562.471	562.471	∞
100	131.177	380.502	912.961	-53.246	592.131	647.972	-338.459
200	266.685	510.860	679.186	-33.665	576.382	710.109	-185.458
250	344.340	578.658	652.264	-18.401	569.018	744.392	-155.529
298.15	419.786	645.776	645.776	0.000	562.471	778.780	-136.436
300	422.648	648.382	645.784	0.779	562.229	780.120	-135.828
350	497.904	719.243	651.209	23.812	556.207	816.926	-121.917
400	567.729	790.355	664.159	50.478	550.993	854.525	-111.587
450	631.024	860.945	682.111	80.475	546.489	892.743	-103.625
500	687.622	930.417	703.479	113.469	542.592	931.454	-97.306
600	782.494	1064.516	752.576	187.164	536.274	1009.854	-87.914
700	857.383	1190.984	806.267	269.302	531.688	1089.176	-81.274
800	917.271	1309.525	861.847	358.142	528.637	1169.030	-76.328
900	965.918	1420.468	917.820	452.383	526.922	1249.176	-72.499
1000	1005.979	1524.377	973.337	551.040	526.362	1329.466	-69.443
1100	1039.339	1621.869	1027.909	653.356	526.730	1409.778	-66.943
1200	1067.369	1713.540	1081.264	758.731	527.869	1489.998	-64.857
1300	1091.102	1799.938	1133.256	866.687	529.570	1570.114	-63.087
1400	1111.329	1881.557	1183.818	976.835	531.682	1650.086	-61.564
1500	1128.674	1958.837	1232.933	1088.857	534.116	1729.899	-60.239
1600	1143.629	2032.169	1280.613	1202.490	536.720	1809.531	-59.074
1700	1156.593	2101.899	1326.890	1317.516	539.412	1888.969	-58.040
1800	1167.887	2168.335	1371.806	1433.753	542.105	1968.325	-57.118
1900	1177.772	2231.750	1415.410	1551.047	544.765	2047.468	-56.288
2000	1186.464	2292.388	1457.754	1669.268	547.330	2126.506	-55.537
2100	1194.139	2350.465	1498.891	1788.306	549.708	2205.402	-54.855
2200	1200.945	2406.177	1538.874	1908.066	551.900	2284.191	-54.232
2300	1207.003	2459.697	1577.754	2028.470	553.902	2362.886	-53.662
2400	1212.415	2511.183	1615.581	2149.445	555.629	2441.438	-53.135
2500	1217.267	2560.777	1652.403	2270.934	557.097	2520.063	-52.653
2600	1221.632	2608.605	1688.266	2392.883	558.264	2598.491	-52.203
2700	1225.571	2654.785	1723.212	2515.246	559.135	2676.972	-51.788
2800	1229.136	2699.422	1757.284	2637.984	559.681	2755.450	-51.402
2900	1232.373	2742.611	1790.521	2761.062	559.865	2833.850	-51.042
3000	1235.319	2784.441	1822.958	2884.449	559.742	2912.283	-50.706
3100	1238.007	2824.991	1854.631	3008.118	559.219	2990.629	-50.391
3200	1240.467	2864.336	1885.572	3132.043	558.346	3069.090	-50.097
3300	1242.722	2902.542	1915.813	3256.204	557.103	3147.633	-49.822
3400	1244.795	2939.672	1945.383	3380.581	555.455	3226.110	-49.562
3500	1246.704	2975.784	1974.310	3505.158	553.408	3304.619	-49.318
3600	1248.466	3010.929	2002.619	3629.917	550.990	3383.304	-49.089
3700	1250.096	3045.159	2030.335	3754.846	548.164	3462.078	-48.875
3800	1251.605	3078.517	2057.482	3879.932	544.897	3540.863	-48.672
3900	1253.007	3111.046	2084.081	4005.164	541.239	3619.673	-48.479
4000	1254.309	3142.786	2110.153	4130.531	537.172	3698.755	-48.300
4100	1255.522	3173.773	2135.719	4256.023	532.651	3777.853	-48.129
4200	1256.654	3204.042	2160.796	4381.632	527.711	3857.055	-47.969
4300	1257.711	3233.624	2185.403	4507.351	522.336	3936.268	-47.815
4400	1258.699	3262.550	2209.556	4633.172	516.536	4015.725	-47.672
4500	1259.625	3290.847	2233.272	4759.089	510.330	4095.386	-47.537
4600	1260.494	3318.542	2256.565	4885.095	503.652	4175.203	-47.410
4700	1261.310	3345.659	2279.449	5011.186	496.523	4255.028	-47.288
4800	1262.077	3372.222	2301.940	5137.356	488.998	4335.142	-47.175
4900	1262.800	3398.253	2324.049	5263.600	480.986	4415.247	-47.066
5000	1263.481	3423.772	2345.789	5389.914	472.603	4495.751	-46.966

3.604. Benzo[*rst*]phenanthro[10,1,2-*cde*]pentaphene



Other names: Dinaphtho[1,2,3-*cd*,1',2',3'-*lm*]perylene

Formula: C₃₄H₁₈

Mass: 426.507 g/mol

CAS Number: 188-84-1

Point Group: C_{2h}

Length: 20.15 Å

Width: 9.200 Å

Breadth: 3.888 Å

L/B Ratio: 2.190

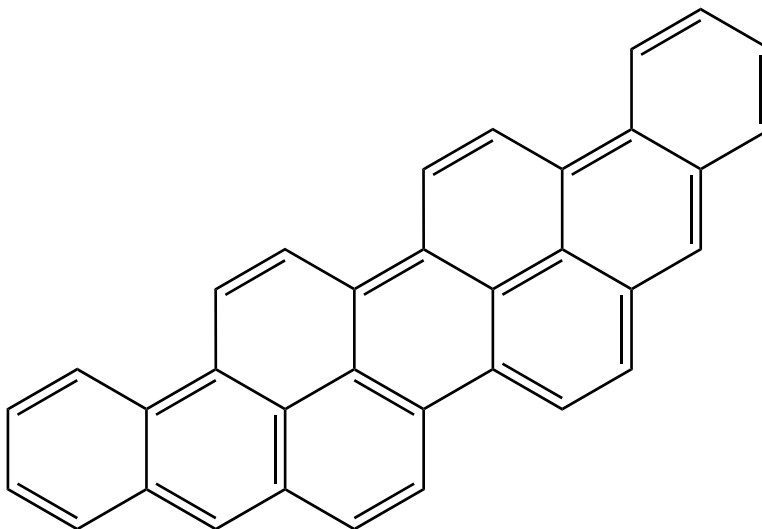
Cartesian coordinates:

C	7.3542	-1.4049	0.0000	C	-1.7723	2.2319	0.0000	H	7.4060	2.0087	0.0000
C	7.8675	-0.0872	0.0000	C	-3.1142	2.0445	0.0000	H	5.5880	-2.6392	0.0000
C	7.0169	0.9841	0.0000	C	-3.6782	0.7267	0.0000	H	5.1414	2.9076	0.0000
C	6.0031	-1.6197	0.0000	C	-4.7241	-1.8930	0.0000	H	2.8759	3.8315	0.0000
C	5.0935	-0.5276	0.0000	C	-2.8187	-0.3779	0.0000	H	0.4183	3.4872	0.0000
C	5.6080	0.7863	0.0000	C	-3.3594	-1.7019	0.0000	H	1.3424	-3.2452	0.0000
C	4.7240	1.8930	0.0000	C	-2.4482	-2.8222	0.0000	H	3.8107	-2.8971	0.0000
C	3.3594	1.7019	0.0000	C	-1.1126	-2.6329	0.0000	H	-1.3424	3.2453	0.0000
C	2.4482	2.8221	0.0000	C	-0.5343	-1.3106	0.0000	H	-3.8107	2.8971	0.0000
C	1.1127	2.6329	0.0000	C	-1.3944	-0.1906	0.0000	H	-5.1413	-2.9077	0.0000
C	0.5344	1.3107	0.0000	C	-5.6080	-0.7864	0.0000	H	-2.8757	-3.8315	0.0000
C	1.3944	0.1906	0.0000	C	-5.0935	0.5276	0.0000	H	-0.4181	-3.4871	0.0000
C	0.8624	-1.1218	0.0000	C	-6.0031	1.6197	0.0000	H	-5.5879	2.6392	0.0000
C	1.7723	-2.2319	0.0000	C	-7.3542	1.4049	0.0000	H	-8.0515	2.2490	0.0000
C	3.1141	-2.0445	0.0000	C	-7.8676	0.0872	0.0000	H	-8.9522	-0.0622	0.0000
C	3.6781	-0.7267	0.0000	C	-7.0169	-0.9842	0.0000	H	-7.4059	-2.0088	0.0000
C	2.8187	0.3779	0.0000	H	8.0514	-2.2491	0.0000				
C	-0.8623	1.1219	0.0000	H	8.9521	0.0624	0.0000				

Table 3.604: Table of thermodynamic data as a function of temperature for Benzo[*rst*]phenanthro[10,1,2-*cde*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-61.544	547.261	547.261	∞
100	133.002	382.094	916.776	-53.468	576.699	632.381	-330.315
200	267.771	513.412	682.177	-33.753	561.084	694.301	-181.329
250	345.241	581.434	655.191	-18.439	553.770	728.451	-152.198
298.15	420.455	648.691	648.691	0.000	547.261	762.701	-133.619
300	423.308	651.301	648.699	0.780	547.021	764.036	-133.028
350	498.308	722.244	654.131	23.840	541.025	800.693	-119.494
400	567.908	793.395	667.094	50.521	535.825	838.141	-109.448
450	631.025	863.995	685.058	80.522	531.325	876.207	-101.705
500	687.493	933.460	706.436	113.512	527.425	914.766	-95.563
600	782.224	1067.522	755.545	187.186	521.087	992.863	-86.435
700	857.069	1193.944	809.238	269.294	516.471	1071.887	-79.984
800	916.962	1312.442	864.814	358.103	513.389	1151.447	-75.180
900	965.633	1423.350	920.780	452.314	511.643	1231.304	-71.462
1000	1005.725	1527.231	976.287	550.944	511.056	1311.307	-68.494
1100	1039.115	1624.700	1030.849	653.236	511.400	1391.334	-66.068
1200	1067.174	1716.352	1084.194	758.590	512.519	1471.272	-64.042
1300	1090.931	1802.736	1136.176	866.528	514.201	1551.107	-62.323
1400	1111.180	1884.343	1186.729	976.660	516.297	1630.800	-60.845
1500	1128.542	1961.614	1235.835	1088.667	518.717	1710.335	-59.558
1600	1143.513	2034.938	1283.508	1202.288	521.309	1789.690	-58.426
1700	1156.490	2104.661	1329.777	1317.304	523.990	1868.851	-57.422
1800	1167.795	2171.092	1374.686	1433.531	526.673	1947.932	-56.526
1900	1177.690	2234.502	1418.283	1550.816	529.324	2026.799	-55.719
2000	1186.390	2295.136	1460.621	1669.029	531.881	2105.562	-54.991
2100	1194.072	2353.210	1501.753	1788.060	534.252	2184.183	-54.327
2200	1200.884	2408.918	1541.730	1907.814	536.438	2262.698	-53.722
2300	1206.947	2462.436	1580.605	2028.212	538.434	2341.119	-53.167
2400	1212.364	2513.920	1618.427	2149.182	540.156	2419.397	-52.656
2500	1217.220	2563.511	1655.245	2270.666	541.619	2497.749	-52.187
2600	1221.589	2611.338	1691.103	2392.610	542.781	2575.904	-51.749
2700	1225.531	2657.516	1726.046	2514.969	543.649	2654.111	-51.346
2800	1229.099	2702.151	1760.114	2637.704	544.190	2732.316	-50.971
2900	1232.339	2745.340	1793.347	2760.778	544.371	2810.444	-50.621
3000	1235.287	2787.168	1825.781	2884.162	544.245	2888.604	-50.294
3100	1237.977	2827.718	1857.451	3007.827	543.718	2966.677	-49.987
3200	1240.439	2867.061	1888.389	3131.750	542.843	3044.865	-49.701
3300	1242.696	2905.267	1918.628	3255.908	541.597	3123.136	-49.434
3400	1244.770	2942.396	1948.195	3380.283	539.946	3201.340	-49.182
3500	1246.681	2978.507	1977.119	3504.857	537.897	3279.577	-48.944
3600	1248.445	3013.652	2005.426	3629.614	535.477	3357.990	-48.722
3700	1250.075	3047.880	2033.140	3754.541	532.648	3436.492	-48.514
3800	1251.586	3081.238	2060.284	3879.625	529.379	3515.005	-48.316
3900	1252.988	3113.767	2086.881	4004.855	525.720	3593.542	-48.129
4000	1254.292	3145.507	2112.952	4130.219	521.651	3672.353	-47.955
4100	1255.506	3176.493	2138.515	4255.710	517.128	3751.178	-47.790
4200	1256.638	3206.762	2163.591	4381.318	512.187	3830.108	-47.633
4300	1257.696	3236.344	2188.196	4507.035	506.811	3909.050	-47.485
4400	1258.685	3265.269	2212.347	4632.855	501.009	3988.234	-47.345
4500	1259.612	3293.566	2236.061	4758.770	494.801	4067.623	-47.215
4600	1260.481	3321.260	2259.353	4884.775	488.122	4147.169	-47.092
4700	1261.297	3348.377	2282.236	5010.864	480.992	4226.722	-46.974
4800	1262.065	3374.940	2304.725	5137.033	473.465	4306.564	-46.864
4900	1262.788	3400.970	2326.832	5263.276	465.452	4386.397	-46.759
5000	1263.469	3426.489	2348.571	5389.589	457.069	4466.629	-46.662

3.605. Anthra[9,1,2-*cde*]benzo[*rst*]pentaphene



Other names: Dinaphtho[1,2,3-*cd*,3',2',1'-*lm*]perylene

Formula: C₃₄H₁₈

Mass: 426.507 g/mol

CAS Number: 188-87-4

Point Group: C_{2v}

Length: 20.16 Å

Width: 9.209 Å

Breadth: 3.884 Å

L/B Ratio: 2.189

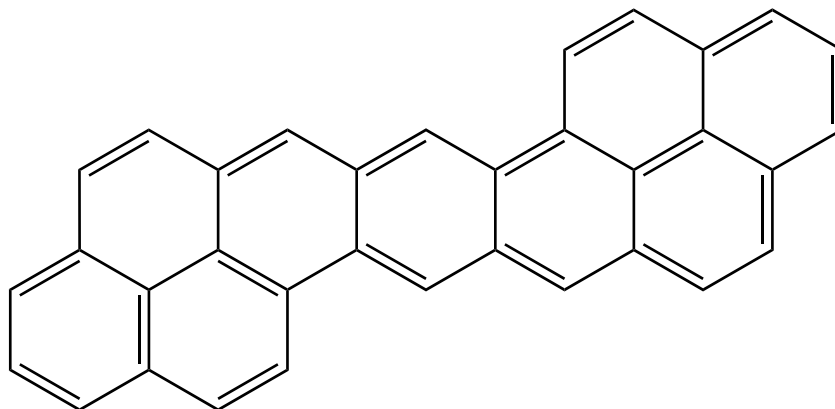
Cartesian coordinates:

C	7.1032	-2.0295	0.0000	C	-1.4562	2.8097	0.0000	H	7.6064	1.3458	0.0000
C	7.7859	-0.7939	0.0000	C	-2.8028	2.8159	0.0000	H	5.1866	-3.0175	0.0000
C	7.0838	0.3825	0.0000	C	-3.5582	1.5821	0.0000	H	5.4828	2.5390	0.0000
C	5.7334	-2.0622	0.0000	C	-4.9320	1.5897	0.0000	H	3.3631	3.7582	0.0000
C	4.9801	-0.8601	0.0000	C	-2.8422	0.3406	0.0000	H	0.8855	3.7514	0.0000
C	5.6639	0.3723	0.0000	C	-3.5460	-0.8696	0.0000	H	0.8922	-3.0452	0.0000
C	4.9318	1.5902	0.0000	C	-2.8148	-2.0960	0.0000	H	3.3886	-3.0354	0.0000
C	3.5580	1.5824	0.0000	C	-1.4555	-2.0996	0.0000	H	-0.8858	3.7513	0.0000
C	2.8025	2.8161	0.0000	C	-0.7127	-0.8793	0.0000	H	-3.3635	3.7579	0.0000
C	1.4560	2.8098	0.0000	C	-1.4090	0.3427	0.0000	H	-5.4830	2.5384	0.0000
C	0.6970	1.5779	0.0000	C	-4.9800	-0.8607	0.0000	H	-3.3882	-3.0358	0.0000
C	1.4090	0.3428	0.0000	C	-5.6639	0.3717	0.0000	H	-0.8919	-3.0453	0.0000
C	0.7128	-0.8792	0.0000	C	-7.0839	0.3818	0.0000	H	-7.6066	1.3450	0.0000
C	1.4557	-2.0995	0.0000	C	-7.7859	-0.7948	0.0000	H	-8.8807	-0.7892	0.0000
C	2.8150	-2.0957	0.0000	C	-7.1030	-2.0303	0.0000	H	-7.6801	-2.9607	0.0000
C	3.5460	-0.8693	0.0000	C	-5.7332	-2.0628	0.0000	H	-5.1863	-3.0181	0.0000
C	2.8422	0.3409	0.0000	H	7.6804	-2.9599	0.0000				
C	-0.6972	1.5778	0.0000	H	8.8808	-0.7882	0.0000				

Table 3.605: Table of thermodynamic data as a function of temperature for Anthra[9,1,2-*cde*]benzo[*rst*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-61.246	543.143	543.143	∞
100	131.880	375.644	909.053	-53.341	572.708	629.035	-328.567
200	267.125	506.347	674.906	-33.712	557.007	691.637	-180.633
250	344.824	574.249	647.948	-18.425	549.666	726.143	-151.716
298.15	420.268	641.453	641.453	0.000	543.143	760.741	-133.276
300	423.129	644.061	641.461	0.780	542.902	762.089	-132.689
350	498.337	714.993	646.891	23.836	536.903	799.109	-119.258
400	568.094	786.159	659.853	50.522	531.708	836.919	-109.288
450	631.321	856.787	677.819	80.536	527.221	875.345	-101.605
500	687.859	926.287	699.202	113.543	523.338	914.264	-95.511
600	782.652	1060.423	748.327	187.257	517.039	993.075	-86.453
700	857.505	1186.912	802.042	269.409	512.467	1072.806	-80.052
800	917.381	1305.468	857.642	358.260	509.427	1153.066	-75.286
900	966.027	1416.424	913.633	452.512	507.723	1233.617	-71.596
1000	1006.091	1520.344	969.164	551.181	507.174	1314.311	-68.651
1100	1039.453	1617.847	1023.749	653.507	507.553	1395.026	-66.243
1200	1067.485	1709.527	1077.116	758.894	508.704	1475.648	-64.232
1300	1091.217	1795.935	1129.118	866.861	510.416	1556.164	-62.526
1400	1111.442	1877.562	1179.691	977.021	512.539	1636.536	-61.059
1500	1128.783	1954.850	1228.815	1089.054	514.985	1716.748	-59.781
1600	1143.735	2028.189	1276.503	1202.698	517.600	1796.778	-58.658
1700	1156.695	2097.926	1322.788	1317.734	520.302	1876.613	-57.660
1800	1167.984	2164.368	1367.711	1433.981	523.005	1956.367	-56.771
1900	1177.864	2227.788	1411.322	1551.284	525.674	2035.907	-55.970
2000	1186.552	2288.430	1453.673	1669.514	528.248	2115.340	-55.246
2100	1194.222	2346.511	1494.816	1788.561	530.635	2194.632	-54.587
2200	1201.023	2402.227	1534.804	1908.330	532.835	2273.816	-53.986
2300	1207.077	2455.750	1573.689	2028.740	534.844	2352.906	-53.435
2400	1212.485	2507.240	1611.521	2149.724	536.578	2431.852	-52.927
2500	1217.334	2556.836	1648.348	2271.219	538.054	2510.872	-52.461
2600	1221.695	2604.667	1684.215	2393.174	539.227	2589.694	-52.027
2700	1225.631	2650.849	1719.166	2515.544	540.105	2668.568	-51.625
2800	1229.193	2695.488	1753.242	2638.288	540.656	2747.440	-51.253
2900	1232.426	2738.679	1786.482	2761.371	540.845	2826.233	-50.905
3000	1235.370	2780.511	1818.923	2884.763	540.728	2905.059	-50.581
3100	1238.056	2821.063	1850.599	3008.437	540.210	2983.798	-50.276
3200	1240.513	2860.409	1881.544	3132.367	539.342	3062.652	-49.992
3300	1242.766	2898.616	1911.788	3256.532	538.103	3141.588	-49.726
3400	1244.837	2935.748	1941.361	3380.914	536.459	3220.457	-49.475
3500	1246.744	2971.860	1970.291	3505.494	534.416	3299.359	-49.239
3600	1248.504	3007.007	1998.602	3630.258	532.003	3378.436	-49.019
3700	1250.132	3041.237	2026.321	3755.191	529.180	3457.602	-48.812
3800	1251.640	3074.597	2053.470	3880.280	525.916	3536.780	-48.615
3900	1253.040	3107.127	2080.072	4005.515	522.262	3615.981	-48.430
4000	1254.341	3138.868	2106.146	4130.885	518.198	3695.455	-48.257
4100	1255.553	3169.856	2131.714	4256.380	513.680	3774.945	-48.092
4200	1256.683	3200.125	2156.794	4381.993	508.744	3854.539	-47.937
4300	1257.738	3229.708	2181.402	4507.714	503.371	3934.143	-47.789
4400	1258.726	3258.634	2205.557	4633.538	497.574	4013.991	-47.651
4500	1259.651	3286.932	2229.275	4759.458	491.370	4094.044	-47.521
4600	1260.519	3314.627	2252.569	4885.466	484.695	4174.253	-47.399
4700	1261.334	3341.745	2275.456	5011.560	477.568	4254.469	-47.282
4800	1262.100	3368.309	2297.948	5137.732	470.046	4334.974	-47.173
4900	1262.822	3394.340	2320.058	5263.978	462.036	4415.470	-47.069
5000	1263.502	3419.859	2341.800	5390.295	453.655	4496.366	-46.972

3.606. Dinaphtho[2,1,8-jkl:2',1',8'-uva]pentacene



Formula: C₃₄H₁₈
Mass: 426.507 g/mol
CAS Number: 123795-83-5
Point Group: C_{2h}

Length: 20.12 Å
Width: 9.625 Å
Breadth: 3.888 Å
L/B Ratio: 2.090

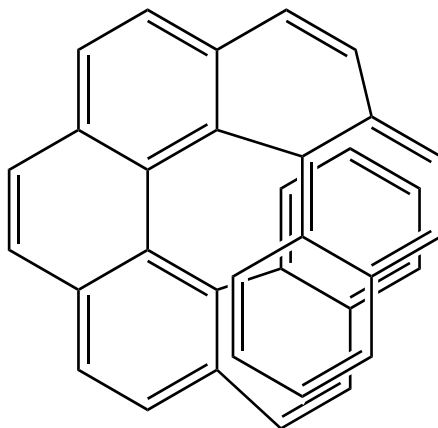
Cartesian coordinates:

C	5.6833	-2.3317	0.0000	C	-3.7240	0.2712	0.0000	H	1.7075	-3.0529	0.0000
C	4.3787	-2.6662	0.0000	C	-5.1132	-0.0710	0.0000	H	0.6468	2.4137	0.0000
C	3.3373	-1.6573	0.0000	C	-5.5022	-1.4259	0.0000	H	-0.6467	-2.4137	0.0000
C	2.0125	-1.9990	0.0000	C	-4.4916	-2.4378	0.0000	H	-1.7075	3.0529	0.0000
C	0.9958	-0.9941	0.0000	C	-3.1740	-2.1013	0.0000	H	-4.0655	3.7167	0.0000
C	1.3598	0.3802	0.0000	C	-2.7579	-0.7338	0.0000	H	-6.4648	3.1003	0.0000
C	0.3560	1.3505	0.0000	C	6.1044	-0.9460	0.0000	H	-8.2166	1.3752	0.0000
C	-0.3559	-1.3506	0.0000	C	7.4462	-0.5957	0.0000	H	-8.8893	-1.0103	0.0000
C	-1.3597	-0.3803	0.0000	C	7.8247	0.7534	0.0000	H	-7.1739	-2.8057	0.0000
C	-0.9957	0.9940	0.0000	C	6.8738	1.7518	0.0000	H	-4.8037	-3.4884	0.0000
C	-2.0125	1.9990	0.0000	C	5.1132	0.0710	0.0000	H	-2.3886	-2.8729	0.0000
C	-3.3373	1.6573	0.0000	C	5.5021	1.4259	0.0000	H	8.2166	-1.3751	0.0000
C	-4.3787	2.6661	0.0000	C	4.4916	2.4379	0.0000	H	8.8892	1.0105	0.0000
C	-5.6833	2.3317	0.0000	C	3.1740	2.1014	0.0000	H	7.1739	2.8057	0.0000
C	-6.1044	0.9460	0.0000	C	2.7579	0.7338	0.0000	H	4.8037	3.4884	0.0000
C	-7.4462	0.5958	0.0000	C	3.7240	-0.2712	0.0000	H	2.3885	2.8729	0.0000
C	-7.8247	-0.7533	0.0000	H	6.4649	-3.1003	0.0000				
C	-6.8739	-1.7517	0.0000	H	4.0656	-3.7168	0.0000				

Table 3.606: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1,8-*ijkl*:2',1',8'-*uva*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-60.668	537.677	537.677	∞
100	128.543	374.610	904.122	-52.951	567.632	624.062	-325.970
200	265.272	503.341	671.329	-33.598	551.656	686.887	-179.393
250	343.728	570.916	644.448	-18.383	544.243	721.552	-150.757
298.15	419.580	637.966	637.966	0.000	537.677	756.315	-132.501
300	422.452	640.571	637.974	0.779	537.435	757.669	-131.919
350	497.849	711.414	643.397	23.806	531.407	794.866	-118.625
400	567.679	782.521	656.345	50.470	526.191	832.857	-108.758
450	630.932	853.102	674.294	80.464	521.683	871.466	-101.155
500	687.486	922.562	695.659	113.452	517.781	910.571	-95.125
600	782.325	1056.633	744.748	187.131	511.447	989.757	-86.164
700	857.249	1183.077	798.429	269.253	506.846	1069.869	-79.833
800	917.208	1301.604	853.999	358.083	503.785	1150.515	-75.119
900	965.931	1412.544	909.964	452.322	502.067	1231.453	-71.470
1000	1006.060	1516.458	965.474	550.984	501.512	1312.535	-68.558
1100	1039.472	1613.960	1020.042	653.310	501.891	1393.639	-66.177
1200	1067.542	1705.644	1073.393	758.701	503.045	1474.649	-64.188
1300	1091.300	1792.057	1125.384	866.675	504.765	1555.553	-62.502
1400	1111.543	1873.692	1175.946	976.844	506.897	1636.313	-61.050
1500	1128.896	1950.987	1225.062	1088.888	509.353	1716.912	-59.787
1600	1143.854	2024.333	1272.744	1202.543	511.980	1797.328	-58.676
1700	1156.816	2094.077	1319.023	1317.592	514.694	1877.548	-57.689
1800	1168.106	2160.526	1363.942	1433.851	517.409	1957.687	-56.809
1900	1177.985	2223.953	1407.549	1551.166	520.091	2037.610	-56.017
2000	1186.669	2284.601	1449.897	1669.408	522.676	2117.427	-55.300
2100	1194.337	2342.688	1491.037	1788.466	525.075	2197.101	-54.649
2200	1201.134	2398.409	1531.024	1908.246	527.286	2276.667	-54.054
2300	1207.183	2451.937	1569.908	2028.668	529.307	2356.139	-53.508
2400	1212.587	2503.431	1607.738	2149.662	531.051	2435.466	-53.005
2500	1217.432	2553.031	1644.564	2271.167	532.536	2514.867	-52.544
2600	1221.789	2600.866	1680.431	2393.132	533.719	2594.069	-52.114
2700	1225.720	2647.051	1715.381	2515.510	534.606	2673.323	-51.717
2800	1229.278	2691.693	1749.457	2638.263	535.166	2752.574	-51.349
2900	1232.508	2734.888	1782.696	2761.355	535.364	2831.747	-51.004
3000	1235.448	2776.722	1815.137	2884.755	535.255	2910.952	-50.683
3100	1238.130	2817.276	1846.813	3008.436	534.744	2990.069	-50.381
3200	1240.584	2856.625	1877.758	3132.374	533.883	3069.301	-50.100
3300	1242.834	2894.835	1908.002	3256.546	532.652	3148.616	-49.837
3400	1244.902	2931.968	1937.575	3380.934	531.014	3227.863	-49.589
3500	1246.806	2968.082	1966.505	3505.521	528.977	3307.143	-49.355
3600	1248.564	3003.231	1994.817	3630.291	526.570	3386.597	-49.137
3700	1250.189	3037.463	2022.536	3755.229	523.753	3466.142	-48.932
3800	1251.695	3070.823	2049.685	3880.324	520.495	3545.696	-48.738
3900	1253.092	3103.355	2076.287	4005.565	516.846	3625.275	-48.554
4000	1254.391	3135.097	2102.362	4130.940	512.787	3705.126	-48.383
4100	1255.601	3166.086	2127.930	4256.440	508.274	3784.993	-48.220
4200	1256.729	3196.357	2153.010	4382.057	503.343	3864.964	-48.067
4300	1257.783	3225.941	2177.619	4507.783	497.975	3944.945	-47.921
4400	1258.769	3254.868	2201.775	4633.611	492.182	4025.170	-47.784
4500	1259.692	3283.167	2225.492	4759.535	485.982	4105.599	-47.656
4600	1260.558	3310.863	2248.787	4885.548	479.311	4186.184	-47.535
4700	1261.372	3337.982	2271.674	5011.645	472.188	4266.777	-47.419
4800	1262.137	3364.546	2294.167	5137.821	464.669	4347.658	-47.311
4900	1262.857	3390.578	2316.278	5264.071	456.663	4428.531	-47.208
5000	1263.536	3416.098	2338.020	5390.391	448.286	4509.802	-47.113

3.607. Naphtho[2,1-c:7,8-c']diphenanthrene



Formula: $C_{34}H_{20}$
Mass: 428.523 g/mol
CAS Number: 20495-12-9
Point Group: C_2

Length: 11.42 Å
Width: 10.52 Å
Breadth: 8.497 Å
L/B Ratio: 1.085

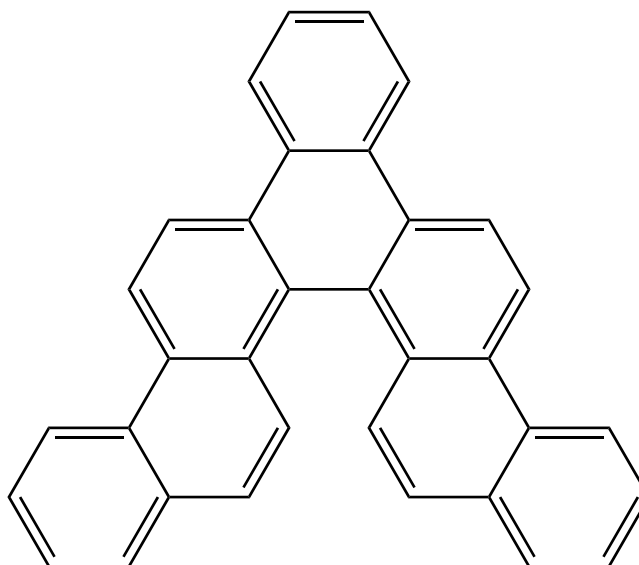
Cartesian coordinates:

C	-0.0243	1.0355	-2.2537	C	0.5774	2.0620	-2.9420	H	0.6976	4.5748	0.8434
C	0.1112	1.1998	1.1194	C	2.8219	-1.3594	-1.9420	H	-1.7667	4.5646	0.4641
C	0.7185	0.0854	1.8154	C	1.9535	2.0191	-3.2255	H	-3.8409	3.3613	0.2453
C	-0.0254	-1.0355	2.2536	C	0.1316	3.6365	0.8254	H	-5.0845	1.2048	0.0800
C	0.1099	-1.2001	-1.1198	C	-1.2087	3.6295	0.5874	H	-5.0857	-1.1997	-0.0810
C	0.7185	-0.0862	-1.8157	C	-1.9011	2.3927	0.4501	H	-3.8442	-3.3574	-0.2449
C	2.0773	0.1587	2.1848	C	-1.1999	1.1746	0.5191	H	-1.7713	-4.5629	-0.4637
C	2.6896	-0.9221	2.8602	C	-3.3140	2.4003	0.2498	H	0.6930	-4.5756	-0.8430
C	1.9509	-2.0203	3.2272	C	-3.9899	1.2271	0.1279	H	2.4204	-2.8575	3.7535
C	0.5749	-2.0620	2.9432	C	-3.2710	0.0017	-0.0004	H	3.8920	-1.3719	-2.1771
C	2.0773	-0.1608	-2.1848	C	-1.8662	0.0009	-0.0002	H	-1.1021	-1.0794	2.0456
C	0.8024	-2.4197	-1.1295	C	-3.9912	-1.2231	-0.1286	H	-0.0173	-2.9208	3.2758
C	2.1889	-2.4671	-1.4842	C	-3.3163	-2.3970	-0.2498	H	2.7246	-3.4159	-1.3650
C	0.1279	-3.6369	-0.8254	C	-1.9035	-2.3908	-0.4500	H	3.7572	-0.8629	3.1006
C	0.8049	2.4187	1.1291	C	-1.2011	-1.1735	-0.5193	H	3.8936	1.3675	2.1760
C	2.1916	2.4645	1.4833	C	-1.2124	-3.6284	-0.5872	H	2.4241	2.8562	-3.7509
C	2.8234	1.3562	1.9414	H	2.7285	3.4125	1.3633	H	-0.0135	2.9220	-3.2739
C	2.6909	0.9198	-2.8592	H	3.7585	0.8597	-3.0993	H	-1.1011	1.0798	-2.0466

Table 3.607: Table of thermodynamic data as a function of temperature for Naphtho[2,1-c:7,8-c']diphenanthrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-64.200	664.356	664.356	∞
100	140.304	378.745	936.679	-55.793	696.936	763.026	-398.555
200	279.252	516.265	692.064	-35.160	679.546	836.074	-218.356
250	359.614	587.153	663.958	-19.201	671.480	876.141	-183.056
298.15	437.715	657.190	657.190	0.000	664.356	916.224	-160.515
300	440.676	659.907	657.199	0.813	664.094	917.785	-159.797
350	518.444	733.739	662.852	24.811	657.588	960.597	-143.358
400	590.432	807.740	676.341	52.560	651.999	1004.264	-131.141
450	655.551	881.112	695.026	83.739	647.216	1048.590	-121.715
500	713.689	953.250	717.254	117.998	643.124	1093.438	-114.228
600	811.064	1092.333	768.282	194.431	636.614	1184.150	-103.087
700	888.004	1223.363	824.033	279.531	632.052	1275.800	-95.199
800	949.700	1346.112	881.706	371.525	629.202	1367.964	-89.317
900	999.991	1460.972	939.759	469.092	627.839	1460.387	-84.757
1000	1041.554	1568.550	997.317	571.233	627.759	1552.907	-81.114
1100	1076.278	1669.497	1053.883	677.175	628.715	1645.395	-78.132
1200	1105.539	1764.436	1109.180	786.307	630.532	1737.735	-75.640
1300	1130.373	1853.933	1163.060	898.136	632.985	1829.909	-73.525
1400	1151.584	1938.499	1215.456	1012.261	635.910	1921.881	-71.705
1500	1169.802	2018.587	1266.352	1128.353	639.206	2013.634	-70.120
1600	1185.535	2094.599	1315.762	1246.138	642.712	2105.146	-68.725
1700	1199.189	2166.891	1363.720	1365.390	646.336	2196.405	-67.486
1800	1211.096	2235.779	1410.269	1485.918	649.986	2287.530	-66.381
1900	1221.527	2301.545	1455.461	1607.560	653.622	2378.386	-65.385
2000	1230.707	2364.440	1499.349	1730.182	657.177	2469.086	-64.485
2100	1238.818	2424.687	1541.988	1853.666	660.556	2559.593	-63.665
2200	1246.013	2482.486	1583.433	1977.915	663.756	2649.948	-62.916
2300	1252.422	2538.017	1623.738	2102.843	666.772	2740.160	-62.230
2400	1258.149	2591.443	1662.953	2228.376	669.516	2830.186	-61.596
2500	1263.287	2642.909	1701.128	2354.453	672.003	2920.244	-61.014
2600	1267.910	2692.548	1738.311	2481.017	674.186	3010.063	-60.472
2700	1272.083	2740.479	1774.546	2608.020	676.073	3099.894	-59.970
2800	1275.861	2786.811	1809.875	2735.420	677.632	3189.688	-59.503
2900	1279.291	2831.643	1844.340	2863.180	678.824	3279.366	-59.067
3000	1282.414	2875.067	1877.977	2991.268	679.706	3369.042	-58.659
3100	1285.265	2917.164	1910.824	3119.654	680.180	3458.598	-58.276
3200	1287.874	2958.011	1942.914	3248.313	680.299	3548.237	-57.918
3300	1290.266	2997.678	1974.278	3377.222	680.039	3637.927	-57.582
3400	1292.465	3036.230	2004.948	3506.360	679.367	3727.522	-57.265
3500	1294.491	3073.725	2034.951	3635.709	678.289	3817.121	-56.966
3600	1296.361	3110.218	2064.315	3765.253	676.831	3906.864	-56.686
3700	1298.090	3145.761	2093.065	3894.977	674.954	3996.676	-56.422
3800	1299.693	3180.401	2121.225	4024.867	672.626	4086.468	-56.171
3900	1301.180	3214.180	2148.818	4154.911	669.899	4176.263	-55.934
4000	1302.563	3247.141	2175.866	4285.099	666.751	4266.307	-55.711
4100	1303.851	3279.321	2202.389	4415.421	663.138	4356.342	-55.499
4200	1305.052	3310.755	2228.406	4545.867	659.096	4446.460	-55.299
4300	1306.174	3341.477	2253.935	4676.429	654.606	4536.566	-55.107
4400	1307.224	3371.517	2278.995	4807.099	649.681	4626.898	-54.927
4500	1308.208	3400.905	2303.601	4937.871	644.337	4717.416	-54.757
4600	1309.130	3429.668	2327.769	5068.739	638.510	4808.068	-54.596
4700	1309.997	3457.832	2351.514	5199.695	632.219	4898.709	-54.442
4800	1310.812	3485.421	2374.851	5330.736	625.522	4989.620	-54.297
4900	1311.579	3512.457	2397.792	5461.856	618.326	5080.507	-54.158
5000	1312.303	3538.962	2420.351	5593.051	610.748	5171.780	-54.028

3.608. Phenanthro[2,1-f]picene



Formula: $C_{34}H_{20}$
Mass: 428.523 g/mol
CAS Number: 111381-82-9
Point Group: C_2

Length: 16.09 Å
Width: 13.72 Å
Breadth: 6.264 Å
L/B Ratio: 1.172

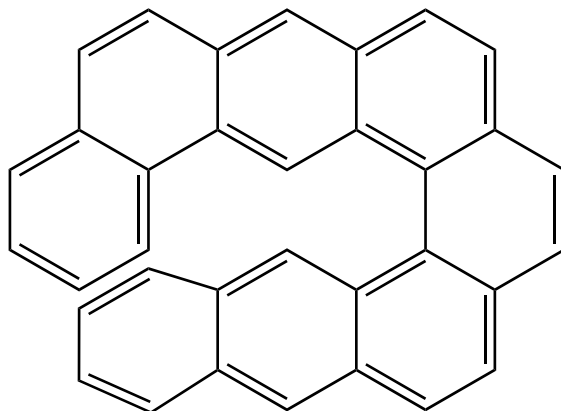
Cartesian coordinates:

C	5.0557	1.4663	0.4702	C	-1.5530	0.2477	0.1931	H	-3.5896	4.4961	1.4687
C	3.7264	1.4037	-0.0061	C	-2.8986	0.2379	-0.2071	H	-5.4598	0.5953	-1.0120
C	3.2036	2.5033	-0.7079	C	-3.4482	-0.9371	-0.7781	H	-1.4946	3.2791	1.8124
C	4.0059	3.6471	-0.9181	C	-2.7123	-2.0867	-0.8218	H	0.0564	1.3231	-1.3626
C	5.2942	3.6873	-0.4392	C	-1.0773	1.3660	0.9593	H	-3.1582	-3.0295	-1.1738
C	5.8228	2.5873	0.2597	C	-1.8654	2.4395	1.2130	H	-4.4895	-0.9113	-1.1339
C	1.8648	2.4402	-1.2137	C	-3.2045	2.5018	0.7080	H	2.2825	-4.5710	0.9990
C	1.0773	1.3661	-0.9606	C	-3.7267	1.4023	0.0056	H	1.1306	-6.7263	0.5206
C	1.5533	0.2481	-0.1942	C	-4.0076	3.6449	0.9196	H	-1.1294	-6.7267	-0.5171
C	2.8988	0.2388	0.2062	C	-5.2959	3.6844	0.4408	H	-2.2814	-4.5719	-0.9976
C	0.7255	-0.8920	0.0695	C	-5.8240	2.5848	-0.2592	H	4.4900	-0.9099	1.1334
C	1.3558	-2.0941	0.4110	C	-5.0561	1.4643	-0.4705	H	3.1595	-3.0284	1.1730
C	2.7132	-2.0857	0.8210	C	1.2732	-4.5819	0.5600	H	-0.0563	1.3234	1.3612
C	3.4489	-0.9361	0.7771	C	0.6385	-5.7757	0.2905	H	1.4937	3.2797	-1.8129
C	-0.7249	-0.8922	-0.0704	C	-0.6373	-5.7760	-0.2880	H	3.5870	4.4990	-1.4657
C	-1.3549	-2.0946	-0.4118	C	-1.2721	-4.5824	-0.5586	H	5.9173	4.5732	-0.5988
C	-0.6495	-3.3533	-0.2657	H	-6.8518	2.6286	-0.6337	H	6.8507	2.6314	0.6342
C	0.6506	-3.3530	0.2659	H	-5.9199	4.5696	0.6015	H	5.4596	0.5975	1.0120

Table 3.608: Table of thermodynamic data as a function of temperature for Phenanthro[2,1-f]picene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-64.408	598.460	598.460	∞
100	142.457	389.000	947.224	-55.822	631.012	696.076	-363.585
200	279.275	527.450	702.787	-35.068	613.743	768.034	-200.586
250	358.606	598.227	674.766	-19.135	605.651	807.544	-168.724
298.15	436.004	668.023	668.023	0.000	598.460	847.099	-148.405
300	438.943	670.729	668.031	0.809	598.195	848.639	-147.758
350	516.264	744.257	673.661	24.709	591.591	890.918	-132.959
400	588.018	817.950	687.094	52.342	585.886	934.067	-121.974
450	653.046	891.031	705.702	83.398	580.980	977.890	-113.508
500	711.187	962.904	727.841	117.532	576.762	1022.249	-106.791
600	808.697	1101.541	778.675	193.720	570.008	1112.018	-96.808
700	885.827	1232.221	834.231	278.592	565.218	1202.765	-89.750
800	947.711	1354.692	891.719	370.378	562.160	1294.058	-84.492
900	998.173	1469.327	949.599	467.755	560.607	1385.635	-80.418
1000	1039.891	1576.721	1006.999	569.722	560.352	1477.329	-77.166
1100	1074.754	1677.517	1063.421	675.505	561.149	1569.008	-74.504
1200	1104.142	1772.328	1118.586	784.491	562.821	1660.552	-72.280
1300	1129.092	1861.719	1172.345	896.186	565.140	1751.943	-70.392
1400	1150.407	1946.194	1224.631	1010.188	567.943	1843.141	-68.767
1500	1168.721	2026.204	1275.426	1126.168	571.126	1934.128	-67.351
1600	1184.539	2102.149	1324.743	1243.850	574.528	2024.882	-66.104
1700	1198.270	2174.382	1372.614	1363.006	578.056	2115.389	-64.997
1800	1210.248	2243.220	1419.084	1483.445	581.617	2205.767	-64.008
1900	1220.743	2308.942	1464.202	1605.006	585.172	2295.882	-63.117
2000	1229.979	2371.798	1508.022	1727.552	588.652	2385.844	-62.311
2100	1238.142	2432.011	1550.598	1850.966	591.960	2475.617	-61.576
2200	1245.385	2489.780	1591.984	1975.150	595.096	2565.241	-60.905
2300	1251.836	2545.284	1632.233	2100.017	598.051	2654.724	-60.289
2400	1257.603	2598.686	1671.397	2225.494	600.738	2744.025	-59.721
2500	1262.776	2650.131	1709.523	2351.518	603.172	2833.361	-59.199
2600	1267.431	2699.750	1746.660	2478.032	605.306	2922.458	-58.712
2700	1271.634	2747.663	1782.852	2604.989	607.147	3011.569	-58.261
2800	1275.439	2793.979	1818.142	2732.346	608.662	3100.647	-57.842
2900	1278.894	2838.797	1852.568	2860.065	609.813	3189.608	-57.450
3000	1282.040	2882.208	1886.170	2988.114	610.656	3278.569	-57.084
3100	1284.912	2924.293	1918.982	3116.464	611.094	3367.412	-56.739
3200	1287.540	2965.130	1951.039	3245.088	611.179	3456.338	-56.418
3300	1289.950	3004.787	1982.373	3373.965	610.887	3545.317	-56.117
3400	1292.166	3043.329	2013.014	3503.072	610.184	3634.202	-55.832
3500	1294.207	3080.815	2042.989	3632.392	609.076	3723.091	-55.563
3600	1296.091	3117.301	2072.327	3761.908	607.590	3812.126	-55.311
3700	1297.833	3152.837	2101.052	3891.605	605.688	3901.230	-55.074
3800	1299.448	3187.469	2129.188	4021.471	603.335	3990.315	-54.850
3900	1300.947	3221.243	2156.758	4151.491	600.583	4079.403	-54.636
4000	1302.340	3254.198	2183.784	4281.656	597.412	4168.741	-54.437
4100	1303.638	3286.372	2210.285	4411.956	593.778	4258.071	-54.247
4200	1304.849	3317.801	2236.282	4542.381	589.715	4347.483	-54.068
4300	1305.980	3348.518	2261.792	4672.923	585.205	4436.885	-53.896
4400	1307.038	3378.555	2286.833	4803.575	580.261	4526.513	-53.735
4500	1308.029	3407.939	2311.421	4934.329	574.899	4616.328	-53.584
4600	1308.959	3436.698	2335.572	5065.178	569.055	4706.276	-53.440
4700	1309.832	3464.858	2359.301	5196.118	562.747	4796.214	-53.303
4800	1310.654	3492.443	2382.622	5327.143	556.033	4886.424	-53.174
4900	1311.427	3519.476	2405.548	5458.248	548.822	4976.608	-53.050
5000	1312.156	3545.978	2428.092	5589.427	541.229	5067.180	-52.935

3.609. Benzo[*j*]benzo[2,1-*a*:3,4-*a'*]dianthracene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 122961-15-3
Point Group: C₁

Length: 14.13 Å
Width: 12.26 Å
Breadth: 7.882 Å
L/B Ratio: 1.152

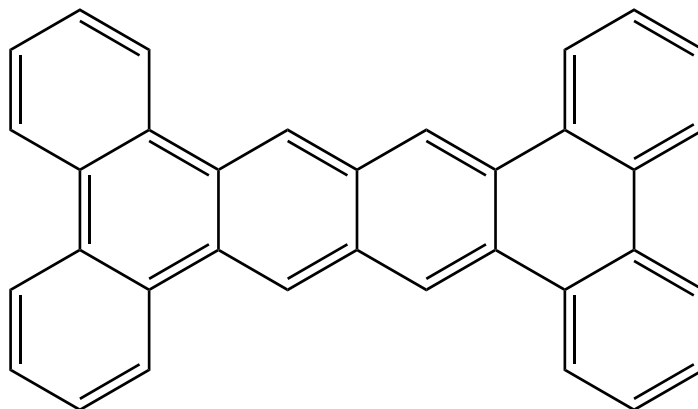
Cartesian coordinates:

C	-0.0136	4.8094	0.6815	C	-0.5965	-1.8408	0.2360	H	2.0700	3.8879	3.1990
C	-0.6569	3.5594	0.4301	C	-0.2408	-3.0430	0.8989	H	0.9898	1.6850	2.7936
C	-0.2856	2.4261	1.1913	C	-1.2672	-3.9684	1.2979	H	3.7390	-3.7959	1.3493
C	0.7107	2.5669	2.2055	C	-2.5481	-3.7613	0.9210	H	5.5381	-2.4115	0.3449
C	1.3036	3.7748	2.4252	C	0.4250	-1.0793	-0.3409	H	0.1785	-0.1853	-0.9401
C	0.9392	4.9097	1.6515	C	1.7695	-1.4205	-0.1890	H	1.3660	-4.2877	1.6339
C	-0.8926	1.1845	0.9332	C	2.1150	-2.5684	0.5635	H	-3.3301	-4.4964	1.1443
C	-1.8462	1.0406	-0.0672	C	1.1041	-3.3728	1.0876	H	-0.9754	-4.8604	1.8636
C	-2.2852	2.2091	-0.7582	C	2.8255	-0.6217	-0.7832	H	-5.6067	-1.2323	-1.4100
C	-1.6725	3.4340	-0.5319	C	4.1671	-0.9907	-0.5837	H	-4.9477	-3.2678	-0.1334
C	-2.5029	-0.2319	-0.3394	C	4.4818	-2.1547	0.2044	H	-3.7172	3.0223	-2.1960
C	-3.7544	-0.1845	-0.9706	C	3.5027	-2.9081	0.7515	H	-5.0972	0.9535	-2.2593
C	-4.1741	1.0031	-1.6701	C	2.5357	0.5206	-1.5550	H	-0.5992	0.3172	1.5414
C	-3.4356	2.1313	-1.6235	C	3.5523	1.2669	-2.1112	H	-1.9993	4.3219	-1.0873
C	-2.0032	-1.5120	0.0661	C	4.8898	0.8962	-1.9116	H	1.4811	0.8031	-1.6990
C	-2.9291	-2.5540	0.2384	C	5.1950	-0.2171	-1.1578	H	3.3198	2.1530	-2.7107
C	-4.2492	-2.4326	-0.2589	H	6.2390	-0.5102	-0.9987	H	1.4365	5.8648	1.8498
C	-4.6228	-1.3020	-0.9322	H	5.6893	1.4967	-2.3575	H	-0.3045	5.6796	0.0825

Table 3.609: Table of thermodynamic data as a function of temperature for Benzo[*j*]benzo[2,1-*a*:3,4-*a'*]dianthracene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	–64.306	604.781	604.781	∞
100	140.683	396.866	953.931	–55.706	637.448	701.726	–366.536
200	278.820	534.445	709.791	–35.069	620.062	772.954	–201.871
250	358.670	605.181	681.761	–19.145	611.962	812.116	–169.679
298.15	436.334	675.014	675.014	0.000	604.781	851.335	–149.147
300	439.280	677.722	675.022	0.810	604.517	852.863	–148.494
350	516.695	751.311	680.657	24.729	597.932	894.790	–133.537
400	588.449	825.062	694.101	52.384	592.249	937.585	–122.434
450	653.441	898.192	712.724	83.461	587.363	981.051	–113.875
500	711.539	970.105	734.878	117.613	583.164	1025.051	–107.084
600	808.999	1108.801	785.745	193.833	576.442	1114.097	–96.989
700	886.130	1239.526	841.332	278.736	571.683	1204.116	–89.850
800	948.042	1362.039	898.847	370.554	568.657	1294.676	–84.532
900	998.538	1476.715	956.754	467.965	567.138	1385.516	–80.412
1000	1040.284	1584.150	1014.180	569.970	566.921	1476.469	–77.121
1100	1075.166	1684.984	1070.626	675.794	567.759	1567.403	–74.428
1200	1104.562	1779.832	1125.814	784.821	569.472	1658.199	–72.178
1300	1129.511	1869.256	1179.596	896.558	571.833	1748.838	–70.268
1400	1150.819	1953.762	1231.903	1010.602	574.677	1839.281	–68.623
1500	1169.121	2033.800	1282.719	1126.622	577.901	1929.509	–67.190
1600	1184.924	2109.770	1332.055	1244.343	581.342	2019.502	–65.929
1700	1198.639	2182.027	1379.946	1363.537	584.908	2109.246	–64.808
1800	1210.599	2250.885	1426.434	1484.013	588.505	2198.859	–63.808
1900	1221.076	2316.626	1471.569	1605.608	592.095	2288.206	–62.906
2000	1230.296	2379.498	1515.405	1728.186	595.607	2377.399	–62.090
2100	1238.441	2439.726	1557.996	1851.631	598.946	2466.401	–61.347
2200	1245.668	2497.508	1599.397	1975.844	602.110	2555.253	–60.668
2300	1252.104	2553.025	1639.660	2100.738	605.093	2643.963	–60.045
2400	1257.856	2606.438	1678.837	2226.242	607.806	2732.489	–59.470
2500	1263.015	2657.892	1716.976	2352.290	610.265	2821.049	–58.941
2600	1267.657	2707.521	1754.126	2478.827	612.422	2909.370	–58.449
2700	1271.847	2755.442	1790.329	2605.806	614.285	2997.704	–57.993
2800	1275.641	2801.766	1825.629	2733.184	615.820	3086.003	–57.569
2900	1279.086	2846.591	1860.066	2860.923	616.992	3174.185	–57.172
3000	1282.222	2890.008	1893.678	2988.991	617.853	3262.366	–56.802
3100	1285.085	2932.099	1926.500	3117.358	618.309	3350.429	–56.453
3200	1287.704	2972.941	1958.566	3245.999	618.410	3438.574	–56.128
3300	1290.106	3012.603	1989.908	3374.892	618.134	3526.772	–55.823
3400	1292.314	3051.150	2020.557	3504.014	617.447	3614.875	–55.535
3500	1294.348	3088.640	2050.541	3633.349	616.354	3702.981	–55.263
3600	1296.226	3125.130	2079.886	3762.879	614.881	3791.234	–55.008
3700	1297.962	3160.669	2108.618	3892.589	612.992	3879.555	–54.768
3800	1299.571	3195.305	2136.761	4022.467	610.652	3967.856	–54.541
3900	1301.064	3229.082	2164.338	4152.499	607.912	4056.161	–54.325
4000	1302.453	3262.040	2191.370	4282.676	604.753	4144.715	–54.123
4100	1303.746	3294.217	2217.878	4412.987	601.130	4233.260	–53.931
4200	1304.952	3325.648	2243.881	4543.422	597.077	4321.888	–53.749
4300	1306.079	3356.368	2269.397	4673.975	592.578	4410.505	–53.576
4400	1307.133	3386.406	2294.443	4804.636	587.643	4499.348	–53.413
4500	1308.120	3415.792	2319.037	4935.399	582.290	4588.377	–53.259
4600	1309.047	3444.554	2343.193	5066.258	576.455	4677.540	–53.114
4700	1309.917	3472.716	2366.927	5197.206	570.155	4766.693	–52.975
4800	1310.735	3500.303	2390.253	5328.239	563.450	4856.116	–52.844
4900	1311.505	3527.337	2413.184	5459.352	556.247	4945.515	–52.719
5000	1312.231	3553.840	2435.732	5590.539	548.662	5035.300	–52.602

3.610. Tetrabenzo[*a,c,j,l*]naphthacene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 215-95-2
Point Group: D_{2h}

Length: 16.57 Å
Width: 11.66 Å
Breadth: 3.885 Å
L/B Ratio: 1.422

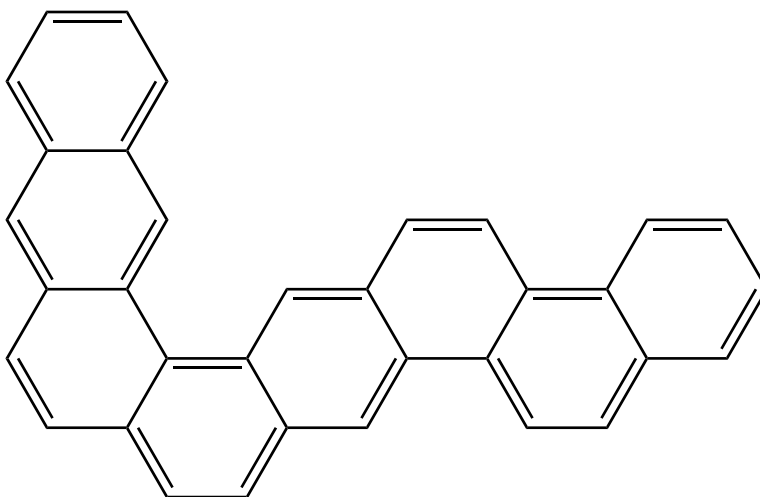
Cartesian coordinates:

C	6.1357	-2.8261	0.0000	C	-1.2356	1.3950	0.0000	H	2.7765	-3.3854	0.0000
C	6.1286	-1.4433	0.0000	C	-1.2345	-1.3959	0.0000	H	4.9328	-4.6223	0.0000
C	3.7310	-2.8371	0.0000	C	-2.4356	-0.7157	0.0000	H	7.0767	0.8909	0.0000
C	4.9292	-3.5276	0.0000	C	-2.4362	0.7138	0.0000	H	7.0825	3.3768	0.0000
C	3.7060	-1.4329	0.0000	C	-3.7048	-1.4360	0.0000	H	4.9290	4.6264	0.0000
C	4.9206	-0.7271	0.0000	C	-4.9200	-0.7312	0.0000	H	2.7738	3.3878	0.0000
C	3.7049	1.4360	0.0000	C	-6.1274	-1.4483	0.0000	H	1.2316	2.4979	0.0000
C	4.9201	0.7312	0.0000	C	-6.1333	-2.8312	0.0000	H	1.2337	-2.4968	0.0000
C	6.1274	1.4483	0.0000	C	-4.9263	-3.5316	0.0000	H	-1.2336	2.4969	0.0000
C	6.1334	2.8312	0.0000	C	-3.7287	-2.8402	0.0000	H	-1.2315	-2.4979	0.0000
C	4.9263	3.5316	0.0000	C	-4.9206	0.7271	0.0000	H	-7.0766	-0.8909	0.0000
C	3.7287	2.8402	0.0000	C	-3.7060	1.4330	0.0000	H	-7.0825	-3.3768	0.0000
C	2.4362	-0.7137	0.0000	C	-3.7312	2.8372	0.0000	H	-4.9290	-4.6264	0.0000
C	2.4356	0.7158	0.0000	C	-4.9294	3.5275	0.0000	H	-2.7737	-3.3877	0.0000
C	1.2345	1.3960	0.0000	C	-6.1359	2.8260	0.0000	H	-2.7767	3.3856	0.0000
C	1.2357	-1.3949	0.0000	C	-6.1286	1.4431	0.0000	H	-4.9331	4.6223	0.0000
C	0.0003	-0.7062	0.0000	H	7.0853	-3.3710	0.0000	H	-7.0855	3.3707	0.0000
C	-0.0003	0.7063	0.0000	H	7.0773	-0.8851	0.0000	H	-7.0773	0.8849	0.0000

Table 3.610: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,c,j,l*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-65.036	565.468	565.468	∞
100	145.842	397.040	956.986	-55.995	597.847	662.107	-345.842
200	279.940	536.937	712.169	-35.046	580.771	733.165	-191.479
250	358.325	607.755	684.176	-19.105	572.688	772.199	-161.339
298.15	435.115	677.445	677.445	0.000	565.468	811.297	-142.133
300	438.036	680.145	677.453	0.808	565.201	812.820	-141.522
350	514.985	753.503	683.071	24.651	558.541	854.632	-127.544
400	586.544	827.011	696.472	52.216	552.767	897.324	-117.176
450	651.495	899.913	715.035	83.195	547.785	940.698	-109.191
500	709.629	971.622	737.120	117.251	543.489	984.617	-102.860
600	807.235	1109.982	787.837	193.287	536.583	1073.529	-93.457
700	884.512	1240.447	843.274	278.021	531.655	1163.443	-86.815
800	946.544	1362.752	900.649	369.683	528.473	1253.922	-81.871
900	997.141	1477.258	958.425	466.950	526.810	1344.699	-78.043
1000	1038.977	1584.550	1015.730	568.820	526.458	1435.606	-74.987
1100	1073.942	1685.263	1072.066	674.517	527.168	1526.506	-72.486
1200	1103.418	1780.008	1127.153	783.426	528.763	1617.279	-70.397
1300	1128.443	1869.343	1180.842	895.052	531.014	1707.905	-68.623
1400	1149.823	1953.773	1233.064	1008.993	533.755	1798.343	-67.096
1500	1168.193	2033.745	1283.800	1124.917	536.882	1888.573	-65.765
1600	1184.061	2109.657	1333.064	1242.548	540.234	1978.575	-64.593
1700	1197.836	2181.863	1380.887	1361.659	543.717	2068.333	-63.551
1800	1209.851	2250.677	1427.312	1482.057	547.237	2157.964	-62.621
1900	1220.380	2316.379	1472.389	1603.580	550.754	2247.334	-61.782
2000	1229.646	2379.217	1516.171	1726.091	554.199	2336.553	-61.023
2100	1237.835	2439.414	1558.712	1849.473	557.475	2425.585	-60.332
2200	1245.102	2497.169	1600.065	1973.627	560.581	2514.470	-59.700
2300	1251.574	2552.661	1640.284	2098.467	563.509	2603.215	-59.120
2400	1257.359	2606.052	1679.419	2223.919	566.171	2691.778	-58.584
2500	1262.549	2657.487	1717.520	2349.919	568.581	2780.378	-58.092
2600	1267.220	2707.098	1754.632	2476.412	570.693	2868.740	-57.633
2700	1271.436	2755.004	1790.801	2603.348	572.514	2957.117	-57.208
2800	1275.254	2801.313	1826.068	2730.686	574.009	3045.461	-56.813
2900	1278.721	2846.125	1860.474	2858.387	575.143	3133.689	-56.443
3000	1281.877	2889.529	1894.056	2986.419	575.969	3221.917	-56.097
3100	1284.758	2931.609	1926.850	3114.753	576.391	3310.028	-55.772
3200	1287.395	2972.441	1958.890	3243.363	576.461	3398.223	-55.469
3300	1289.813	3012.094	1990.208	3372.225	576.155	3486.471	-55.185
3400	1292.036	3050.632	2020.832	3501.319	575.439	3574.626	-54.916
3500	1294.084	3088.115	2050.793	3630.627	574.318	3662.785	-54.663
3600	1295.975	3124.597	2080.117	3760.131	572.820	3751.090	-54.426
3700	1297.723	3160.130	2108.828	3889.817	570.906	3839.464	-54.202
3800	1299.343	3194.760	2136.952	4019.671	568.543	3927.820	-53.991
3900	1300.847	3228.530	2164.510	4149.681	565.781	4016.180	-53.790
4000	1302.245	3261.483	2191.524	4279.837	562.601	4104.789	-53.602
4100	1303.547	3293.655	2218.014	4410.127	558.957	4193.390	-53.423
4200	1304.762	3325.082	2244.000	4540.543	554.885	4282.075	-53.254
4300	1305.897	3355.797	2269.500	4671.077	550.367	4370.749	-53.093
4400	1306.959	3385.831	2294.531	4801.720	545.414	4459.648	-52.942
4500	1307.953	3415.214	2319.110	4932.467	540.044	4548.736	-52.799
4600	1308.886	3443.971	2343.252	5063.309	534.193	4637.957	-52.665
4700	1309.763	3472.130	2366.972	5194.242	527.878	4727.167	-52.535
4800	1310.587	3499.714	2390.285	5325.260	521.157	4816.650	-52.415
4900	1311.363	3526.745	2413.203	5456.358	513.939	4906.107	-52.299
5000	1312.094	3553.246	2435.740	5587.531	506.340	4995.952	-52.191

3.611. Benzo[6,7]phenanthro[4,3-*b*]chrysene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 119123-34-1
Point Group: C₁

Length: 18.87 Å
Width: 12.04 Å
Breadth: 5.147 Å
L/B Ratio: 1.567

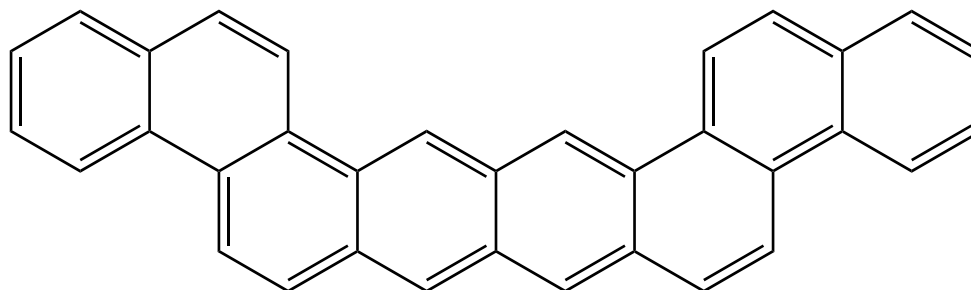
Cartesian coordinates:

C	4.8883	4.0552	-0.6469	C	-1.3822	-2.1015	-0.2856	H	7.4871	2.1048	0.4268
C	6.1998	3.6872	-0.2356	C	0.3457	-0.0190	0.3549	H	2.8783	3.4045	-1.0083
C	6.4800	2.4004	0.1121	C	-1.0303	0.2102	0.3182	H	6.7410	-0.2397	0.6400
C	3.8908	3.1288	-0.6921	C	-1.9150	-0.8379	-0.0356	H	2.1283	1.1252	-0.6665
C	4.1474	1.7705	-0.3234	C	-2.9007	1.7346	0.5735	H	6.0689	-2.5377	0.7791
C	5.4565	1.4029	0.0702	C	-1.5679	1.5057	0.6329	H	4.3486	-4.2931	0.4174
C	5.7187	0.0625	0.3796	C	-3.8198	0.6962	0.1996	H	2.1792	-4.9635	-0.1879
C	3.1290	0.8067	-0.3397	C	-3.3367	-0.5754	-0.0997	H	-0.2256	-4.4746	-0.5811
C	3.3607	-0.5157	0.0322	C	-4.2479	-1.6109	-0.4666	H	-2.0697	-2.9297	-0.5232
C	4.7053	-0.8904	0.3335	C	-5.5858	-1.3760	-0.5330	H	1.0000	0.8145	0.6502
C	5.0357	-2.2761	0.5233	C	-5.2327	0.9565	0.1333	H	-3.3208	2.7245	0.8098
C	4.0955	-3.2291	0.3410	C	-6.1096	-0.0818	-0.2341	H	-0.8715	2.3021	0.9201
C	2.3255	-1.5394	0.0506	C	-7.5025	0.1687	-0.3023	H	-3.8314	-2.6049	-0.6920
C	2.7303	-2.8714	0.0768	C	-7.9977	1.4147	-0.0124	H	-6.2832	-2.1729	-0.8155
C	1.7989	-3.9358	-0.1537	C	-7.1230	2.4569	0.3566	H	-8.1752	-0.6474	-0.5897
C	0.4865	-3.6733	-0.3531	C	-5.7717	2.2337	0.4281	H	-9.0735	1.6111	-0.0643
C	0.8988	-1.2662	0.0430	H	4.6974	5.0966	-0.9258	H	-7.5341	3.4456	0.5852
C	-0.0056	-2.3332	-0.2187	H	6.9777	4.4571	-0.2065	H	-5.0785	3.0389	0.7152

Table 3.611: Table of thermodynamic data as a function of temperature for Benzo[6,7]phenanthro[4,3-*b*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-64.440	584.210	584.210	∞
100	141.664	400.868	958.814	-55.795	616.789	680.666	-355.536
200	279.211	538.945	714.390	-35.089	599.471	751.464	-196.258
250	358.860	609.746	686.348	-19.151	591.385	790.398	-165.141
298.15	436.387	679.599	679.599	0.000	584.210	829.397	-145.304
300	439.328	682.308	679.608	0.810	583.946	830.916	-144.672
350	516.647	755.897	685.243	24.729	577.361	872.614	-130.228
400	588.338	829.636	698.686	52.380	571.674	915.180	-119.508
450	653.290	902.751	717.307	83.450	566.782	958.418	-111.248
500	711.365	974.647	739.458	117.594	562.574	1002.190	-104.696
600	808.801	1113.308	790.316	193.796	555.834	1090.784	-94.959
700	885.922	1244.002	845.891	278.678	551.054	1180.354	-88.077
800	947.831	1366.488	903.394	370.475	548.007	1270.468	-82.951
900	998.328	1481.139	961.289	467.865	546.467	1360.864	-78.981
1000	1040.078	1588.552	1018.702	569.850	546.230	1451.376	-75.811
1100	1074.966	1689.366	1075.137	675.653	547.047	1541.871	-73.216
1200	1104.370	1784.197	1130.313	784.660	548.740	1632.229	-71.048
1300	1129.328	1873.606	1184.084	896.379	551.083	1722.432	-69.207
1400	1150.646	1958.099	1236.381	1010.405	553.909	1812.441	-67.622
1500	1168.958	2038.125	1287.187	1126.408	557.116	1902.236	-66.240
1600	1184.771	2114.085	1336.514	1244.113	560.541	1991.797	-65.024
1700	1198.495	2186.333	1384.396	1363.292	564.092	2081.110	-63.943
1800	1210.464	2255.183	1430.876	1483.754	567.676	2170.293	-62.979
1900	1220.950	2320.917	1476.003	1605.336	571.252	2259.210	-62.109
2000	1230.177	2383.783	1519.832	1727.902	574.752	2347.974	-61.322
2100	1238.331	2444.005	1562.416	1851.336	578.080	2436.549	-60.605
2200	1245.564	2501.782	1603.811	1975.538	581.233	2524.973	-59.949
2300	1252.006	2557.295	1644.068	2100.422	584.206	2613.256	-59.348
2400	1257.764	2610.703	1683.238	2225.916	586.910	2701.355	-58.792
2500	1262.929	2662.154	1721.372	2351.955	589.359	2789.488	-58.282
2600	1267.576	2711.780	1758.516	2478.485	591.509	2877.383	-57.806
2700	1271.771	2759.698	1794.715	2605.455	593.363	2965.291	-57.366
2800	1275.570	2806.019	1830.010	2732.826	594.892	3053.165	-56.956
2900	1279.018	2850.842	1864.443	2860.558	596.056	3140.922	-56.573
3000	1282.158	2894.256	1898.050	2988.619	596.911	3228.678	-56.215
3100	1285.024	2936.346	1930.868	3116.980	597.360	3316.316	-55.878
3200	1287.646	2977.185	1962.930	3245.616	597.456	3404.037	-55.564
3300	1290.052	3016.846	1994.269	3374.502	597.174	3491.810	-55.270
3400	1292.262	3055.391	2024.915	3503.619	596.481	3579.489	-54.991
3500	1294.299	3092.880	2054.895	3632.949	595.383	3667.171	-54.728
3600	1296.179	3129.368	2084.237	3762.474	593.906	3755.000	-54.483
3700	1297.918	3164.906	2112.966	3892.180	592.012	3842.897	-54.251
3800	1299.528	3199.541	2141.106	4022.053	589.667	3930.775	-54.031
3900	1301.024	3233.317	2168.680	4152.082	586.924	4018.656	-53.823
4000	1302.414	3266.274	2195.710	4282.255	583.761	4106.787	-53.628
4100	1303.709	3298.450	2222.215	4412.561	580.133	4194.908	-53.443
4200	1304.917	3329.880	2248.215	4542.993	576.077	4283.113	-53.267
4300	1306.045	3360.599	2273.729	4673.542	571.574	4371.307	-53.100
4400	1307.100	3390.637	2298.773	4804.200	566.636	4459.726	-52.943
4500	1308.089	3420.022	2323.364	4934.960	561.280	4548.333	-52.795
4600	1309.017	3448.783	2347.519	5065.816	555.442	4637.073	-52.655
4700	1309.888	3476.944	2371.250	5196.761	549.139	4725.803	-52.520
4800	1310.707	3504.531	2394.574	5327.792	542.431	4814.803	-52.395
4900	1311.479	3531.564	2417.503	5458.901	535.225	4903.779	-52.274
5000	1312.206	3558.067	2440.050	5590.086	527.638	4993.142	-52.162

3.612. Dinaphtho[2,1-*a*:1',2'-*l*]naphthacene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 126762-84-3
Point Group: C_{2v}

Length: 21.49 Å
Width: 9.528 Å
Breadth: 3.884 Å
L/B Ratio: 2.255

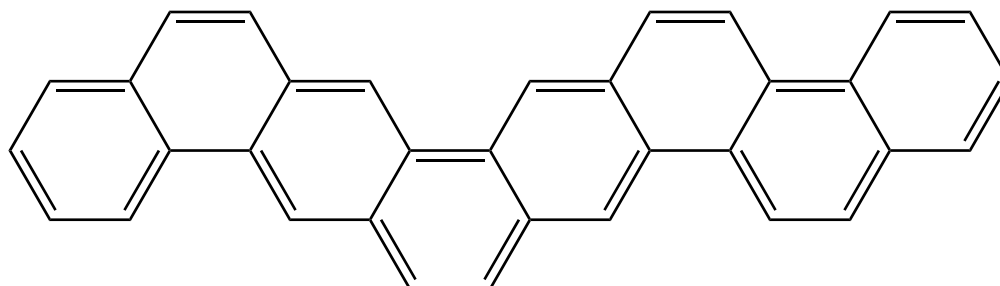
Cartesian coordinates:

C	-8.5881	1.6744	0.0000	C	1.2337	-2.5185	0.0000	H	-7.3767	-1.5228	0.0000
C	-8.5809	0.2638	0.0000	C	1.2309	0.2843	0.0000	H	-7.4021	3.4655	0.0000
C	-7.3943	-0.4223	0.0000	C	2.4348	-0.3965	0.0000	H	-2.7918	2.2667	0.0000
C	-7.4064	2.3696	0.0000	C	2.4307	-1.8265	0.0000	H	-4.9606	3.4890	0.0000
C	-6.1685	1.6785	0.0000	C	3.6892	-2.5303	0.0000	H	-5.8217	-2.3971	0.0000
C	-6.1565	0.2703	0.0000	C	4.8605	-1.8588	0.0000	H	-3.6633	-3.6297	0.0000
C	-3.7495	1.7236	0.0000	C	3.7091	0.3019	0.0000	H	-1.2275	-3.6168	0.0000
C	-4.9346	2.3933	0.0000	C	4.8990	-0.4190	0.0000	H	-1.2332	1.3850	0.0000
C	-3.7094	0.2984	0.0000	C	4.9323	2.3981	0.0000	H	1.2309	-3.6156	0.0000
C	-4.8986	-0.4236	0.0000	C	3.7478	1.7272	0.0000	H	1.2318	1.3862	0.0000
C	-4.8588	-1.8635	0.0000	C	6.1669	1.6844	0.0000	H	3.6668	-3.6262	0.0000
C	-3.6867	-2.5338	0.0000	C	6.1563	0.2762	0.0000	H	5.8240	-2.3915	0.0000
C	-2.4344	-0.3988	0.0000	C	7.3947	-0.4153	0.0000	H	4.9572	3.4938	0.0000
C	-2.4290	-1.8288	0.0000	C	8.5808	0.2720	0.0000	H	2.7896	2.2693	0.0000
C	-1.2312	-2.5197	0.0000	C	8.5865	1.6826	0.0000	H	7.3782	-1.5157	0.0000
C	-1.2312	0.2831	0.0000	C	7.4042	2.3767	0.0000	H	9.5336	-0.2674	0.0000
C	0.0002	-0.4088	0.0000	H	-9.5456	2.2053	0.0000	H	9.5436	2.2144	0.0000
C	0.0009	-1.8284	0.0000	H	-9.5333	-0.2764	0.0000	H	7.3988	3.4726	0.0000

Table 3.612: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1-*a*:1',2'-*l*]naphthacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-64.443	567.875	567.875	∞
100	142.345	393.292	951.275	-55.798	600.451	665.085	-347.398
200	279.212	531.607	706.919	-35.062	583.163	736.623	-192.382
250	358.587	602.379	678.901	-19.131	575.070	775.925	-162.117
298.15	435.830	672.160	672.160	0.000	567.875	815.280	-142.831
300	438.761	674.865	672.168	0.809	567.610	816.813	-142.217
350	515.816	748.346	677.796	24.693	560.990	858.886	-128.179
400	587.308	821.961	691.218	52.297	555.256	901.833	-117.765
450	652.133	894.946	709.809	83.312	550.309	945.457	-109.744
500	710.140	966.716	731.923	117.396	546.042	989.623	-103.383
600	807.565	1105.151	782.695	193.474	539.177	1079.021	-93.935
700	884.760	1235.660	838.180	278.236	534.277	1169.416	-87.261
800	946.773	1357.997	895.595	369.921	531.118	1260.372	-82.292
900	997.377	1472.529	953.406	467.211	529.478	1351.624	-78.445
1000	1039.227	1579.847	1010.741	569.106	529.151	1443.002	-75.373
1100	1074.206	1680.585	1067.105	674.828	529.887	1534.371	-72.860
1200	1103.690	1775.353	1122.216	783.764	531.509	1625.610	-70.760
1300	1128.718	1864.710	1175.927	895.418	533.787	1716.701	-68.976
1400	1150.097	1949.160	1228.170	1009.386	536.555	1807.601	-67.441
1500	1168.461	2029.151	1278.926	1125.337	539.710	1898.292	-66.103
1600	1184.321	2105.080	1328.208	1242.995	543.088	1988.752	-64.925
1700	1198.087	2177.302	1376.048	1362.131	546.596	2078.967	-63.878
1800	1210.091	2246.130	1422.489	1482.554	550.141	2169.054	-62.943
1900	1220.609	2311.844	1467.581	1604.100	553.681	2258.878	-62.100
2000	1229.864	2374.693	1511.377	1726.633	557.149	2348.550	-61.337
2100	1238.043	2434.901	1553.931	1850.037	560.446	2438.034	-60.642
2200	1245.298	2492.665	1595.296	1974.211	563.572	2527.369	-60.006
2300	1251.760	2548.166	1635.527	2099.070	566.519	2616.564	-59.423
2400	1257.536	2601.565	1674.673	2224.540	569.199	2705.577	-58.884
2500	1262.716	2653.007	1712.784	2350.558	571.627	2794.625	-58.389
2600	1267.378	2702.624	1749.906	2477.066	573.755	2883.434	-57.928
2700	1271.586	2750.535	1786.084	2604.018	575.591	2972.259	-57.501
2800	1275.396	2796.850	1821.361	2731.370	577.101	3061.049	-57.103
2900	1278.856	2841.667	1855.775	2859.086	578.249	3149.723	-56.731
3000	1282.005	2885.076	1889.365	2987.131	579.088	3238.397	-56.384
3100	1284.880	2927.160	1922.167	3115.478	579.523	3326.953	-56.058
3200	1287.511	2967.996	1954.215	3244.099	579.604	3415.593	-55.753
3300	1289.924	3007.652	1985.539	3372.973	579.310	3504.285	-55.467
3400	1292.142	3046.193	2016.171	3502.077	578.604	3592.884	-55.197
3500	1294.185	3083.679	2046.138	3631.395	577.494	3681.486	-54.942
3600	1296.070	3120.164	2075.467	3760.909	576.006	3770.235	-54.704
3700	1297.814	3155.699	2104.185	3890.604	574.102	3859.053	-54.479
3800	1299.430	3190.331	2132.314	4020.468	571.747	3947.851	-54.266
3900	1300.930	3224.104	2159.877	4150.487	568.994	4036.654	-54.064
4000	1302.325	3257.059	2186.896	4280.650	565.821	4125.706	-53.875
4100	1303.624	3289.233	2213.392	4410.948	562.186	4214.749	-53.695
4200	1304.836	3320.662	2239.383	4541.372	558.121	4303.875	-53.525
4300	1305.967	3351.379	2264.887	4671.913	553.610	4392.991	-53.363
4400	1307.026	3381.414	2289.923	4802.563	548.664	4482.333	-53.211
4500	1308.018	3410.798	2314.506	4933.316	543.301	4571.862	-53.068
4600	1308.949	3439.557	2338.652	5064.165	537.456	4661.524	-52.932
4700	1309.823	3467.717	2362.376	5195.104	531.147	4751.177	-52.802
4800	1310.645	3495.302	2385.692	5326.128	524.433	4841.100	-52.681
4900	1311.418	3522.335	2408.614	5457.231	517.220	4930.999	-52.564
5000	1312.148	3548.836	2431.155	5588.410	509.627	5021.284	-52.456

3.613. Benzo[*c*]naphtho[2,1-*m*]pentaphene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 119000-41-8
Point Group: C_s

Length: 22.31 Å
Width: 9.169 Å
Breadth: 3.885 Å
L/B Ratio: 2.433

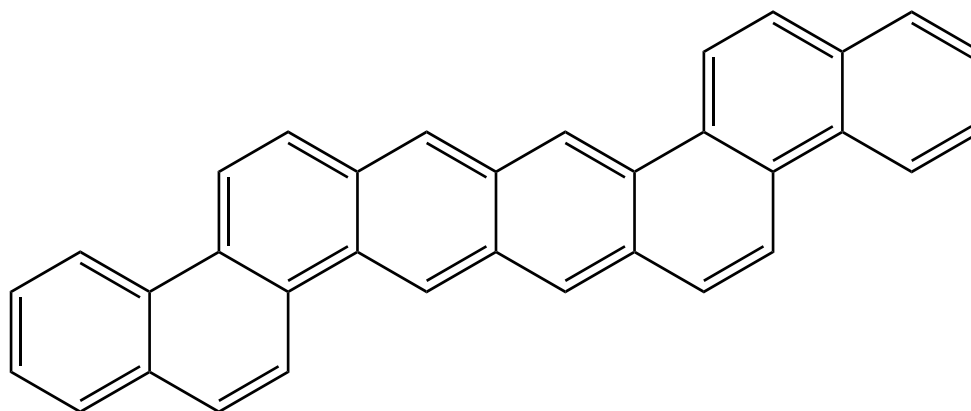
Cartesian coordinates:

C	8.1110	-1.2664	0.0000	C	-1.6719	1.6096	0.0000	H	8.8408	2.0521	0.0000
C	8.8638	-0.1120	0.0000	C	-0.4254	-0.8875	0.0000	H	6.3483	2.2006	0.0000
C	8.2333	1.1414	0.0000	C	-1.8259	-0.8125	0.0000	H	3.9559	-3.2557	0.0000
C	6.8582	1.2249	0.0000	C	-2.4620	0.4499	0.0000	H	6.4357	-3.3624	0.0000
C	6.7031	-1.1976	0.0000	C	-3.9763	-1.9305	0.0000	H	4.5386	2.2791	0.0000
C	6.0692	0.0570	0.0000	C	-2.6229	-2.0045	0.0000	H	1.8870	-1.9536	0.0000
C	4.5607	-2.3417	0.0000	C	-4.6508	-0.6656	0.0000	H	2.4743	3.5824	0.0000
C	5.9116	-2.3998	0.0000	C	-3.9056	0.5129	0.0000	H	-0.0022	3.6973	0.0000
C	3.8748	-1.0758	0.0000	C	-4.5779	1.7733	0.0000	H	-2.1729	2.5911	0.0000
C	4.6213	0.1241	0.0000	C	-5.9352	1.8450	0.0000	H	0.0744	-1.8698	0.0000
C	3.9461	1.3497	0.0000	C	-6.0887	-0.6017	0.0000	H	-4.5968	-2.8400	0.0000
C	2.4767	-1.0225	0.0000	C	-6.7243	0.6541	0.0000	H	-2.1112	-2.9737	0.0000
C	1.8061	0.1984	0.0000	C	-8.1389	0.7237	0.0000	H	-3.9606	2.6849	0.0000
C	2.5544	1.4006	0.0000	C	-8.8894	-0.4252	0.0000	H	-6.4473	2.8140	0.0000
C	1.8660	2.6706	0.0000	C	-8.2570	-1.6845	0.0000	H	-8.6225	1.7072	0.0000
C	0.5190	2.7330	0.0000	C	-6.8878	-1.7715	0.0000	H	-9.9831	-0.3742	0.0000
C	0.3526	0.2640	0.0000	H	8.5994	-2.2475	0.0000	H	-8.8694	-2.5921	0.0000
C	-0.2845	1.5321	0.0000	H	9.9573	-0.1661	0.0000	H	-6.3825	-2.7493	0.0000

Table 3.613: Table of thermodynamic data as a function of temperature for Benzo[*c*]naphtho[2,1-*m*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^{\circ}-H^{\circ}(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-64.404	544.663	544.663	∞
100	142.292	401.674	958.710	-55.704	577.333	641.130	-334.885
200	278.665	539.801	714.789	-34.998	560.015	711.837	-185.909
250	357.902	610.433	686.822	-19.097	551.892	750.732	-156.854
298.15	435.150	680.093	680.093	0.000	544.663	789.703	-138.350
300	438.083	682.793	680.101	0.808	544.397	791.221	-137.761
350	515.228	756.176	685.720	24.660	537.745	832.900	-124.301
400	586.836	829.720	699.126	52.237	531.985	875.457	-114.321
450	651.772	902.656	717.697	83.231	527.016	918.696	-106.637
500	709.876	974.393	739.792	117.301	522.734	962.476	-100.547
600	807.445	1112.794	790.529	193.359	515.850	1051.109	-91.505
700	884.732	1243.291	845.986	278.114	510.943	1140.741	-85.121
800	946.804	1365.629	903.379	369.800	507.785	1230.933	-80.370
900	997.446	1480.167	961.173	467.095	506.150	1321.421	-76.692
1000	1039.319	1587.494	1018.496	568.998	505.831	1412.035	-73.756
1100	1074.311	1688.241	1074.850	674.730	506.577	1502.639	-71.353
1200	1103.801	1783.018	1129.954	783.677	508.210	1593.113	-69.345
1300	1128.831	1872.385	1183.660	895.342	510.499	1683.436	-67.640
1400	1150.209	1956.843	1235.899	1009.321	513.279	1773.568	-66.171
1500	1168.571	2036.841	1286.652	1125.283	516.444	1863.491	-64.891
1600	1184.427	2112.777	1335.932	1242.952	519.833	1953.182	-63.764
1700	1198.188	2185.005	1383.771	1362.099	523.352	2042.626	-62.761
1800	1210.188	2253.839	1430.211	1482.531	526.906	2131.942	-61.866
1900	1220.701	2319.559	1475.302	1604.087	530.456	2220.995	-61.058
2000	1229.951	2382.413	1519.098	1726.629	533.932	2309.895	-60.327
2100	1238.125	2442.624	1561.652	1850.041	537.239	2398.607	-59.661
2200	1245.376	2500.392	1603.018	1974.224	540.373	2487.170	-59.052
2300	1251.833	2555.896	1643.249	2099.090	543.327	2575.592	-58.492
2400	1257.605	2609.298	1682.395	2224.567	546.015	2663.832	-57.976
2500	1262.782	2660.743	1720.506	2350.591	548.448	2752.106	-57.501
2600	1267.440	2710.363	1757.629	2477.106	550.584	2840.142	-57.058
2700	1271.645	2758.276	1793.808	2604.064	552.425	2928.192	-56.648
2800	1275.451	2804.593	1829.085	2731.422	553.941	3016.208	-56.267
2900	1278.908	2849.411	1863.500	2859.143	555.094	3104.108	-55.910
3000	1282.055	2892.822	1897.091	2987.193	555.938	3192.008	-55.577
3100	1284.927	2934.908	1929.894	3115.545	556.378	3279.789	-55.263
3200	1287.556	2975.745	1961.942	3244.171	556.464	3367.654	-54.970
3300	1289.966	3015.403	1993.267	3373.049	556.174	3455.571	-54.696
3400	1292.182	3053.945	2023.899	3502.157	555.473	3543.395	-54.437
3500	1294.223	3091.432	2053.867	3631.479	554.366	3631.222	-54.192
3600	1296.107	3127.919	2083.197	3760.997	552.882	3719.195	-53.963
3700	1297.849	3163.455	2111.915	3890.696	550.981	3807.237	-53.747
3800	1299.464	3198.088	2140.045	4020.562	548.630	3895.260	-53.543
3900	1300.962	3231.862	2167.609	4150.585	545.880	3983.287	-53.349
4000	1302.356	3264.817	2194.629	4280.751	542.710	4071.563	-53.168
4100	1303.653	3296.992	2221.125	4411.053	539.078	4159.831	-52.996
4200	1304.863	3328.421	2247.117	4541.479	535.016	4248.181	-52.833
4300	1305.994	3359.139	2272.622	4672.023	530.508	4336.521	-52.677
4400	1307.052	3389.175	2297.658	4802.676	525.565	4425.087	-52.531
4500	1308.043	3418.559	2322.241	4933.431	520.204	4513.840	-52.394
4600	1308.972	3447.319	2346.388	5064.282	514.361	4602.726	-52.265
4700	1309.845	3475.480	2370.113	5195.223	508.054	4691.602	-52.140
4800	1310.666	3503.065	2393.430	5326.249	501.342	4780.749	-52.024
4900	1311.439	3530.098	2416.352	5457.355	494.132	4869.872	-51.912
5000	1312.168	3556.600	2438.893	5588.536	486.541	4959.381	-51.809

3.614. Dinaphtho[2,1-*a*:2',1'-*j*]naphthacene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 119000-43-0
Point Group: C_{2h}

Length: 22.53 Å
Width: 9.019 Å
Breadth: 3.884 Å
L/B Ratio: 2.497

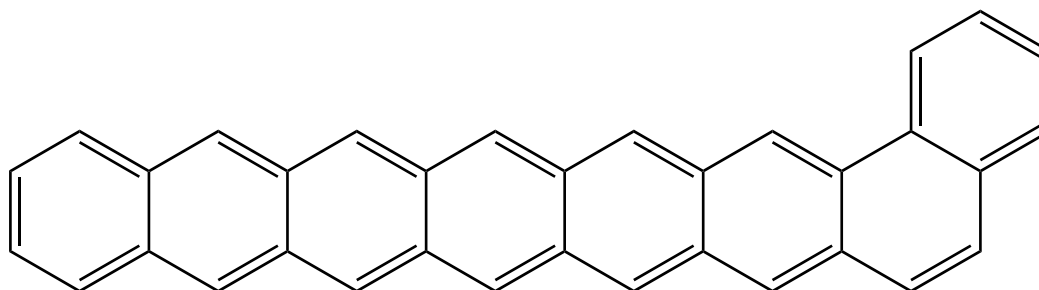
Cartesian coordinates:

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C	9.0230	0.3880	0.0000	C	-1.5626	-1.0201	0.0000	H	6.9988	-2.3673	0.0000
C	8.0710	1.3746	0.0000	C	-2.5388	-0.0406	0.0000	H	6.0149	3.1088	0.0000
C	7.3108	-1.3118	0.0000	C	-2.1501	1.3356	0.0000	H	3.5978	2.5128	0.0000
C	6.3040	-0.3127	0.0000	C	-3.1728	2.3520	0.0000	H	2.8564	-3.4015	0.0000
C	6.6932	1.0408	0.0000	C	-4.4817	2.0204	0.0000	H	5.2663	-2.7926	0.0000
C	5.6961	2.0602	0.0000	C	-3.9540	-0.3705	0.0000	H	1.8597	2.0813	0.0000
C	4.3748	1.7328	0.0000	C	-4.9061	0.6439	0.0000	H	0.5134	-2.7359	0.0000
C	4.9061	-0.6439	0.0000	C	-5.6960	-2.0603	0.0000	H	-0.5134	2.7360	0.0000
C	3.9541	0.3705	0.0000	C	-4.3747	-1.7328	0.0000	H	-1.8597	-2.0812	0.0000
C	3.1728	-2.3519	0.0000	C	-6.6931	-1.0408	0.0000	H	-2.8565	3.4015	0.0000
C	4.4817	-2.0203	0.0000	C	-6.3040	0.3127	0.0000	H	-5.2664	2.7926	0.0000
C	2.1501	-1.3355	0.0000	C	-7.3108	1.3118	0.0000	H	-6.0147	-3.1089	0.0000
C	2.5388	0.0407	0.0000	C	-8.6380	0.9689	0.0000	H	-3.5976	-2.5127	0.0000
C	1.5625	1.0202	0.0000	C	-9.0231	-0.3881	0.0000	H	-6.9988	2.3672	0.0000
C	0.8110	-1.6799	0.0000	C	-8.0710	-1.3747	0.0000	H	-9.4106	1.7447	0.0000
C	-0.1908	-0.6836	0.0000	H	9.4106	-1.7448	0.0000	H	-10.0879	-0.6429	0.0000
C	0.1908	0.6837	0.0000	H	10.0878	0.6427	0.0000	H	-8.3607	-2.4317	0.0000

Table 3.614: Table of thermodynamic data as a function of temperature for Dinaphtho[2,1- α :2',1'- j]naphthacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_f$
0	0.0	0.0	∞	-64.605	565.940	565.940	∞
100	142.665	398.246	956.808	-55.856	598.458	662.597	-346.098
200	279.430	536.712	712.207	-35.099	581.191	733.631	-191.601
250	358.958	607.548	684.159	-19.153	573.114	772.676	-161.438
298.15	436.385	677.410	677.410	0.000	565.940	811.780	-142.218
300	439.322	680.119	677.419	0.810	565.676	813.303	-141.606
350	516.544	753.699	683.053	24.726	559.089	855.111	-127.616
400	588.151	827.420	696.494	52.370	553.394	897.787	-117.237
450	653.039	900.508	715.111	83.429	548.491	941.137	-109.242
500	711.068	972.375	737.256	117.559	544.270	985.021	-102.902
600	808.460	1110.978	788.097	193.728	537.497	1073.845	-93.485
700	885.574	1241.618	843.652	278.576	532.683	1163.651	-86.831
800	947.494	1364.058	901.135	370.338	529.601	1254.006	-81.876
900	998.010	1478.670	959.008	467.696	528.028	1344.647	-78.040
1000	1039.781	1586.050	1016.401	569.650	527.760	1435.408	-74.976
1100	1074.692	1686.838	1072.816	675.424	528.549	1526.154	-72.470
1200	1104.118	1781.646	1127.974	784.406	530.216	1616.766	-70.375
1300	1129.096	1871.035	1181.728	896.100	532.534	1707.225	-68.596
1400	1150.433	1955.511	1234.009	1010.104	535.338	1797.492	-67.064
1500	1168.762	2035.524	1284.800	1126.086	538.525	1887.547	-65.729
1600	1184.591	2111.472	1334.114	1243.773	541.931	1977.369	-64.553
1700	1198.330	2183.709	1381.983	1362.935	545.465	2066.943	-63.508
1800	1210.311	2252.550	1428.450	1483.380	549.033	2156.389	-62.575
1900	1220.809	2318.276	1473.567	1604.948	552.594	2245.570	-61.734
2000	1230.047	2381.135	1517.385	1727.500	556.080	2334.598	-60.972
2100	1238.210	2441.351	1559.960	1850.921	559.396	2423.438	-60.278
2200	1245.452	2499.123	1601.345	1975.111	562.538	2512.128	-59.644
2300	1251.902	2554.630	1641.593	2099.985	565.500	2600.677	-59.062
2400	1257.667	2608.035	1680.756	2225.469	568.193	2689.042	-58.524
2500	1262.838	2659.482	1718.883	2351.499	570.633	2777.443	-58.030
2600	1267.491	2709.104	1756.019	2478.019	572.773	2865.605	-57.570
2700	1271.691	2757.019	1792.211	2604.982	574.620	2953.781	-57.143
2800	1275.494	2803.337	1827.500	2732.344	576.140	3041.923	-56.747
2900	1278.947	2848.157	1861.927	2860.069	577.297	3129.948	-56.375
3000	1282.091	2891.570	1895.528	2988.123	578.146	3217.973	-56.029
3100	1284.961	2933.657	1928.341	3116.478	578.588	3305.880	-55.703
3200	1287.587	2974.495	1960.398	3245.107	578.678	3393.870	-55.398
3300	1289.995	3014.153	1991.732	3373.988	578.391	3481.912	-55.113
3400	1292.209	3052.697	2022.373	3503.100	577.692	3569.860	-54.843
3500	1294.248	3090.184	2052.349	3632.424	576.589	3657.812	-54.589
3600	1296.131	3126.671	2081.687	3761.944	575.107	3745.910	-54.351
3700	1297.872	3162.208	2110.412	3891.646	573.208	3834.077	-54.126
3800	1299.485	3196.842	2138.548	4021.515	570.859	3922.225	-53.914
3900	1300.982	3230.616	2166.119	4151.539	568.111	4010.376	-53.712
4000	1302.374	3263.572	2193.145	4281.707	564.944	4098.777	-53.523
4100	1303.671	3295.747	2219.647	4412.011	561.313	4187.169	-53.344
4200	1304.880	3327.177	2245.644	4542.439	557.253	4275.644	-53.174
4300	1306.010	3357.895	2271.154	4672.984	552.746	4364.108	-53.012
4400	1307.067	3387.932	2296.196	4803.638	547.805	4452.798	-52.860
4500	1308.057	3417.316	2320.784	4934.395	542.446	4541.675	-52.717
4600	1308.986	3446.076	2344.935	5065.248	536.604	4630.686	-52.582
4700	1309.859	3474.237	2368.665	5196.191	530.299	4719.686	-52.452
4800	1310.679	3501.823	2391.986	5327.218	523.588	4808.958	-52.331
4900	1311.452	3528.856	2414.912	5458.325	516.379	4898.204	-52.214
5000	1312.180	3555.358	2437.457	5589.507	508.789	4987.838	-52.107

3.615. Benzo[*a*]heptacene



Formula: $C_{34}H_{20}$
Mass: 428.523 g/mol
CAS Number: 93289-29-3
Point Group: C_1

Length: 23.10 Å
Width: 9.265 Å
Breadth: 3.885 Å
L/B Ratio: 2.493

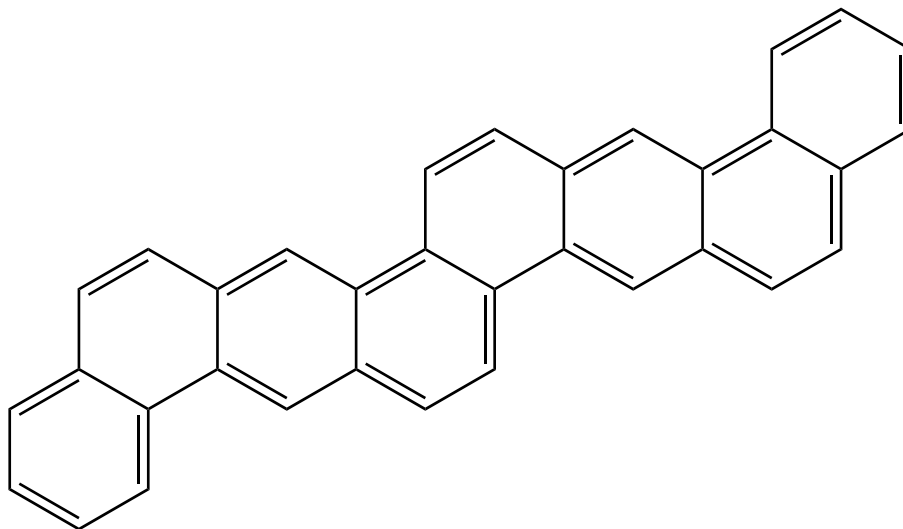
Cartesian coordinates:

C	-9.5173	1.1201	0.0000	C	1.2738	-1.8165	0.0000	H	-8.5881	-2.1811	0.0000
C	-9.6241	-0.3122	0.0000	C	1.4832	0.9913	0.0000	H	-8.2155	2.8147	0.0000
C	-8.5166	-1.0875	0.0000	C	2.6223	0.2153	0.0000	H	-6.1403	-2.3646	0.0000
C	-8.3070	1.7226	0.0000	C	2.5156	-1.2184	0.0000	H	-5.7676	2.6332	0.0000
C	-7.0911	0.9418	0.0000	C	3.7212	-1.9975	0.0000	H	-3.6974	-2.5444	0.0000
C	-7.1983	-0.4957	0.0000	C	3.9293	0.8070	0.0000	H	-3.3250	2.4486	0.0000
C	-6.0663	-1.2700	0.0000	C	5.0599	0.0411	0.0000	H	-1.2557	-2.7260	0.0000
C	-5.8567	1.5397	0.0000	C	4.9496	-1.4009	0.0000	H	-0.8834	2.2661	0.0000
C	-4.6616	0.7571	0.0000	C	6.1617	-2.1970	0.0000	H	1.1862	-2.9101	0.0000
C	-4.7683	-0.6733	0.0000	C	7.3785	-1.6232	0.0000	H	1.5592	2.0857	0.0000
C	-3.6196	-1.4500	0.0000	C	6.3906	0.6410	0.0000	H	3.6309	-3.0911	0.0000
C	-3.4104	1.3548	0.0000	C	7.5289	-0.1829	0.0000	H	4.0144	1.9060	0.0000
C	-2.2339	0.5739	0.0000	C	8.8069	0.3956	0.0000	H	6.0515	-3.2878	0.0000
C	-2.3402	-0.8522	0.0000	C	8.9502	1.7722	0.0000	H	8.2913	-2.2304	0.0000
C	-1.1726	-1.6320	0.0000	C	7.8209	2.5939	0.0000	H	9.6919	-0.2508	0.0000
C	-0.9635	1.1719	0.0000	C	6.5555	2.0344	0.0000	H	9.9491	2.2204	0.0000
C	0.1935	0.3938	0.0000	H	-10.4408	1.7083	0.0000	H	7.9391	3.6823	0.0000
C	0.0870	-1.0342	0.0000	H	-10.6246	-0.7568	0.0000	H	5.6577	2.6715	0.0000

Table 3.615: Table of thermodynamic data as a function of temperature for Benzo[a]heptacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-65.052	644.564	644.564	∞
100	142.935	406.702	969.422	-56.272	676.666	739.959	-386.507
200	281.639	545.949	722.904	-35.391	659.523	810.115	-211.576
250	361.991	617.370	694.622	-19.313	651.577	848.683	-177.319
298.15	439.953	687.816	687.816	0.000	644.564	887.301	-155.448
300	442.905	690.547	687.825	0.817	644.307	888.805	-154.752
350	520.400	764.703	693.504	24.920	637.906	930.077	-138.803
400	592.073	838.945	707.048	52.759	632.407	972.190	-126.952
450	656.895	912.492	725.798	84.012	627.698	1014.951	-117.810
500	714.785	984.759	748.094	118.333	623.666	1058.226	-110.550
600	811.818	1124.008	799.249	194.856	617.248	1145.778	-99.747
700	888.577	1255.139	855.109	280.021	612.751	1234.255	-92.099
800	950.184	1377.959	912.874	372.068	609.954	1323.238	-86.397
900	1000.431	1492.872	971.005	469.681	608.636	1412.473	-81.976
1000	1041.971	1600.495	1028.631	571.864	608.598	1501.801	-78.444
1100	1076.678	1701.482	1085.257	677.848	609.595	1591.093	-75.553
1200	1105.925	1796.454	1140.606	787.018	611.452	1680.232	-73.137
1300	1130.744	1885.982	1194.532	898.885	613.943	1769.203	-71.086
1400	1151.938	1970.575	1246.970	1013.047	616.904	1857.969	-69.320
1500	1170.140	2050.687	1297.905	1129.173	620.235	1946.512	-67.782
1600	1185.855	2126.720	1347.350	1246.992	623.774	2034.814	-66.428
1700	1199.492	2199.031	1395.340	1366.275	627.429	2122.860	-65.226
1800	1211.382	2267.936	1441.918	1486.832	631.108	2210.770	-64.154
1900	1221.798	2333.717	1487.137	1608.502	634.772	2298.410	-63.186
2000	1230.961	2396.625	1531.050	1731.150	638.354	2385.891	-62.312
2100	1239.057	2456.884	1573.713	1854.659	641.757	2473.180	-61.516
2200	1246.239	2514.694	1615.180	1978.931	644.981	2560.314	-60.788
2300	1252.635	2570.235	1655.505	2103.881	648.019	2647.304	-60.121
2400	1258.350	2623.670	1694.739	2229.435	650.783	2734.108	-59.505
2500	1263.476	2675.144	1732.932	2355.531	653.289	2820.944	-58.939
2600	1268.088	2724.790	1770.131	2482.113	655.491	2907.539	-58.412
2700	1272.251	2772.727	1806.382	2609.134	657.396	2994.145	-57.924
2800	1276.020	2819.065	1841.726	2736.550	658.970	3080.714	-57.470
2900	1279.442	2863.903	1876.205	2864.326	660.178	3167.166	-57.046
3000	1282.558	2907.332	1909.855	2992.429	661.075	3253.615	-56.649
3100	1285.401	2949.434	1942.715	3120.829	661.563	3339.945	-56.277
3200	1288.003	2990.285	1974.816	3249.501	661.695	3426.357	-55.928
3300	1290.389	3029.956	2006.192	3378.422	661.448	3512.819	-55.602
3400	1292.582	3068.511	2036.872	3507.572	660.788	3599.187	-55.294
3500	1294.602	3106.009	2066.886	3636.933	659.721	3685.557	-55.003
3600	1296.467	3142.506	2096.259	3766.487	658.273	3772.072	-54.730
3700	1298.191	3178.052	2125.019	3896.221	656.407	3858.655	-54.473
3800	1299.789	3212.694	2153.188	4026.121	654.089	3945.218	-54.230
3900	1301.272	3246.476	2180.790	4156.175	651.371	4031.783	-53.999
4000	1302.651	3279.439	2207.846	4286.372	648.232	4118.598	-53.782
4100	1303.935	3311.620	2234.376	4416.702	644.628	4205.403	-53.576
4200	1305.133	3343.057	2260.400	4547.156	640.594	4292.290	-53.381
4300	1306.252	3373.780	2285.937	4677.726	636.112	4379.166	-53.195
4400	1307.298	3403.823	2311.003	4808.404	631.194	4466.267	-53.020
4500	1308.279	3433.212	2335.616	4939.184	625.858	4553.555	-52.855
4600	1309.199	3461.977	2359.790	5070.058	620.038	4640.976	-52.699
4700	1310.063	3490.142	2383.542	5201.022	613.754	4728.386	-52.549
4800	1310.875	3517.732	2406.884	5332.069	607.063	4816.067	-52.408
4900	1311.640	3544.769	2429.832	5463.195	599.873	4903.722	-52.273
5000	1312.361	3571.275	2452.396	5594.396	592.301	4991.764	-52.148

3.616. Dinaphtho[1,2-*b*:1',2'-*k*]chrysene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 214-13-1
Point Group: C_{2h}

Length: 22.21 Å
Width: 8.734 Å
Breadth: 3.884 Å
L/B Ratio: 2.542

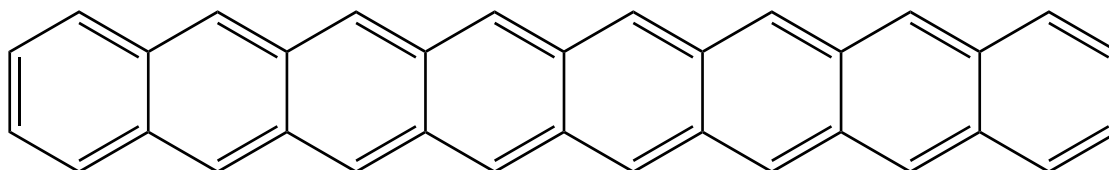
Cartesian coordinates:

C	8.3337	-0.5616	0.0000	C	-1.4488	-2.0872	0.0000	H	8.4138	2.8357	0.0000
C	8.8517	0.7169	0.0000	C	-0.1097	-1.8740	0.0000	H	5.9392	2.5023	0.0000
C	7.9934	1.8248	0.0000	C	-2.3641	-0.9839	0.0000	H	4.6420	-3.3151	0.0000
C	6.6265	1.6423	0.0000	C	-1.8595	0.3384	0.0000	H	7.0944	-2.9402	0.0000
C	6.9402	-0.7635	0.0000	C	-2.7631	1.4103	0.0000	H	4.1460	2.2299	0.0000
C	6.0774	0.3458	0.0000	C	-3.7481	-1.2020	0.0000	H	2.3664	-2.4383	0.0000
C	5.0587	-2.3013	0.0000	C	-4.6409	-0.1352	0.0000	H	1.8576	3.1042	0.0000
C	6.3936	-2.0973	0.0000	C	-4.1369	1.1917	0.0000	H	-0.6005	2.7152	0.0000
C	4.1369	-1.1917	0.0000	C	-5.0587	2.3013	0.0000	H	-1.8576	-3.1041	0.0000
C	4.6409	0.1351	0.0000	C	-6.3936	2.0973	0.0000	H	0.6005	-2.7152	0.0000
C	3.7481	1.2020	0.0000	C	-6.0775	-0.3459	0.0000	H	-2.3664	2.4384	0.0000
C	2.7631	-1.4102	0.0000	C	-6.9402	0.7635	0.0000	H	-4.1459	-2.2299	0.0000
C	1.8595	-0.3383	0.0000	C	-8.3337	0.5616	0.0000	H	-4.6420	3.3151	0.0000
C	2.3641	0.9839	0.0000	C	-8.8518	-0.7169	0.0000	H	-7.0944	2.9402	0.0000
C	1.4488	2.0873	0.0000	C	-7.9934	-1.8248	0.0000	H	-9.0018	1.4304	0.0000
C	0.1098	1.8740	0.0000	C	-6.6266	-1.6423	0.0000	H	-9.9356	-0.8725	0.0000
C	0.4301	-0.5468	0.0000	H	9.0017	-1.4304	0.0000	H	-8.4138	-2.8357	0.0000
C	-0.4301	0.5469	0.0000	H	9.9355	0.8725	0.0000	H	-5.9393	-2.5024	0.0000

Table 3.616: Table of thermodynamic data as a function of temperature for Dinaphtho[1,2-*b*:1',2'-*k*]chrysene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-64.524	547.798	547.798	∞
100	142.694	396.873	954.798	-55.792	580.380	644.656	-336.727
200	279.108	535.278	710.509	-35.046	563.102	715.828	-186.951
250	358.401	606.015	682.504	-19.122	555.002	754.947	-157.734
298.15	435.685	675.766	675.766	0.000	547.798	794.128	-139.125
300	438.618	678.470	675.774	0.809	547.533	795.654	-138.533
350	515.779	751.937	681.400	24.688	540.908	837.547	-124.995
400	587.383	825.554	694.821	52.293	535.175	880.315	-114.955
450	652.302	898.554	713.411	83.314	530.234	923.759	-107.225
500	710.381	970.345	735.527	117.409	525.977	967.744	-101.097
600	807.890	1108.833	786.308	193.515	519.141	1056.777	-91.999
700	885.119	1239.395	841.806	278.312	514.276	1146.801	-85.574
800	947.138	1361.780	899.238	370.034	511.154	1237.381	-80.791
900	997.735	1476.355	957.067	467.360	509.550	1328.252	-77.088
1000	1039.571	1583.710	1014.421	569.289	509.258	1419.245	-74.132
1100	1074.532	1684.480	1070.802	675.046	510.028	1510.227	-71.713
1200	1103.996	1779.276	1125.931	784.013	511.681	1601.075	-69.692
1300	1129.005	1868.657	1179.659	895.697	513.989	1691.772	-67.975
1400	1150.364	1953.127	1231.918	1009.693	516.785	1782.277	-66.496
1500	1168.710	2033.135	1282.689	1125.669	519.965	1872.570	-65.207
1600	1184.552	2109.080	1331.986	1243.351	523.367	1962.631	-64.072
1700	1198.301	2181.315	1379.839	1362.510	526.898	2052.445	-63.063
1800	1210.291	2250.155	1426.293	1482.953	530.463	2142.130	-62.162
1900	1220.795	2315.880	1471.397	1604.519	534.023	2231.551	-61.348
2000	1230.037	2378.739	1515.204	1727.070	537.508	2320.819	-60.612
2100	1238.203	2438.954	1557.768	1850.490	540.822	2409.898	-59.942
2200	1245.448	2496.726	1599.144	1974.680	543.964	2498.827	-59.328
2300	1251.900	2552.233	1639.384	2099.553	546.925	2587.616	-58.765
2400	1257.667	2605.638	1678.539	2225.037	549.619	2676.222	-58.245
2500	1262.839	2657.085	1716.658	2351.067	552.059	2764.862	-57.767
2600	1267.493	2706.707	1753.788	2477.588	554.200	2853.264	-57.322
2700	1271.695	2754.622	1789.974	2604.551	556.047	2941.679	-56.909
2800	1275.498	2800.941	1825.257	2731.913	557.567	3030.061	-56.525
2900	1278.952	2845.761	1859.679	2859.639	558.725	3118.326	-56.166
3000	1282.096	2889.173	1893.275	2987.693	559.574	3206.590	-55.831
3100	1284.966	2931.260	1926.083	3116.049	560.017	3294.737	-55.515
3200	1287.592	2972.098	1958.136	3244.678	560.107	3382.966	-55.220
3300	1290.001	3011.757	1989.466	3373.560	559.820	3471.248	-54.944
3400	1292.214	3050.301	2020.103	3502.672	559.122	3559.436	-54.683
3500	1294.254	3087.789	2050.075	3631.997	558.019	3647.627	-54.437
3600	1296.136	3124.276	2079.410	3761.518	556.538	3735.965	-54.206
3700	1297.877	3159.813	2108.132	3891.219	554.640	3824.372	-53.989
3800	1299.490	3194.446	2136.265	4021.089	552.291	3912.759	-53.784
3900	1300.987	3228.221	2163.833	4151.114	549.544	4001.149	-53.588
4000	1302.379	3261.177	2190.856	4281.283	546.377	4089.790	-53.406
4100	1303.676	3293.352	2217.355	4411.586	542.746	4178.421	-53.233
4200	1304.885	3324.782	2243.350	4542.015	538.687	4267.136	-53.069
4300	1306.015	3355.500	2268.858	4672.561	534.181	4355.840	-52.912
4400	1307.072	3385.537	2293.897	4803.216	529.240	4444.769	-52.765
4500	1308.062	3414.922	2318.483	4933.973	523.881	4533.886	-52.627
4600	1308.991	3443.682	2342.633	5064.826	518.040	4623.136	-52.496
4700	1309.863	3471.843	2366.360	5195.769	511.735	4712.375	-52.371
4800	1310.683	3499.429	2389.679	5326.797	505.025	4801.886	-52.254
4900	1311.456	3526.462	2412.604	5457.904	497.816	4891.372	-52.142
5000	1312.184	3552.964	2435.147	5589.086	490.227	4981.245	-52.038

3.617. Octacene



Formula: C₃₄H₂₀
Mass: 428.523 g/mol
CAS Number: 258-33-3
Point Group: D_{2h}

Length: 23.83 Å
Width: 7.438 Å
Breadth: 3.882 Å
L/B Ratio: 3.203

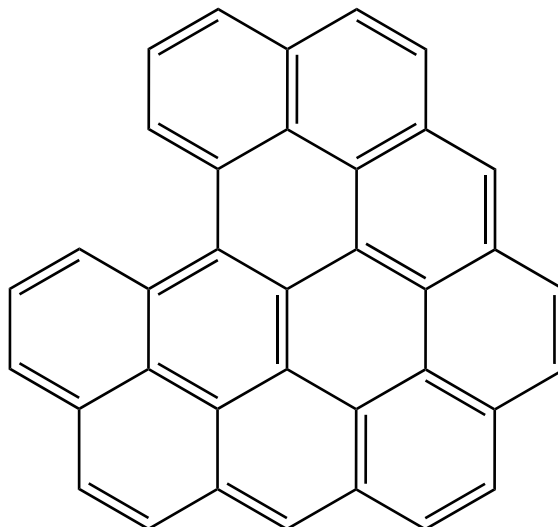
Cartesian coordinates:

C	-9.7454	0.7199	0.0000	C	1.2258	-1.4064	0.0000	H	-8.5750	-2.5046	0.0000
C	-9.7456	-0.7177	0.0000	C	1.2261	1.4061	0.0000	H	-8.5744	2.5066	0.0000
C	-8.5847	-1.4087	0.0000	C	2.4358	0.7168	0.0000	H	-6.1210	-2.5064	0.0000
C	-8.5843	1.4106	0.0000	C	2.4356	-0.7173	0.0000	H	-6.1205	2.5078	0.0000
C	-7.3117	0.7232	0.0000	C	3.6774	-1.4081	0.0000	H	-3.6721	-2.5044	0.0000
C	-7.3118	-0.7215	0.0000	C	3.6777	1.4072	0.0000	H	-3.6715	2.5053	0.0000
C	-6.1291	-1.4093	0.0000	C	4.8732	0.7191	0.0000	H	-1.2241	-2.5033	0.0000
C	-6.1287	1.4107	0.0000	C	4.8730	-0.7202	0.0000	H	-1.2235	2.5036	0.0000
C	-4.8730	0.7202	0.0000	C	6.1287	-1.4107	0.0000	H	1.2235	-2.5036	0.0000
C	-4.8731	-0.7191	0.0000	C	6.1290	1.4093	0.0000	H	1.2241	2.5033	0.0000
C	-3.6779	-1.4073	0.0000	C	7.3119	0.7215	0.0000	H	3.6715	-2.5052	0.0000
C	-3.6775	1.4081	0.0000	C	7.3117	-0.7231	0.0000	H	3.6720	2.5044	0.0000
C	-2.4355	0.7174	0.0000	C	8.5843	-1.4106	0.0000	H	6.1204	-2.5077	0.0000
C	-2.4356	-0.7168	0.0000	C	9.7455	-0.7199	0.0000	H	6.1210	2.5064	0.0000
C	-1.2262	-1.4061	0.0000	C	9.7456	0.7177	0.0000	H	8.5744	-2.5065	0.0000
C	-1.2259	1.4064	0.0000	C	8.5846	1.4087	0.0000	H	10.7105	-1.2370	0.0000
C	0.0002	0.7159	0.0000	H	-10.7105	1.2370	0.0000	H	10.7108	1.2346	0.0000
C	0.0000	-0.7159	0.0000	H	-10.7108	-1.2346	0.0000	H	8.5750	2.5046	0.0000

Table 3.617: Table of thermodynamic data as a function of temperature for Octacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-64.530	690.564	690.564	∞
100	140.895	382.461	943.150	-56.069	722.869	788.587	-411.907
200	280.779	520.710	697.335	-35.325	705.589	861.228	-224.925
250	361.354	591.968	669.101	-19.283	697.607	901.064	-188.263
298.15	439.330	662.306	662.306	0.000	690.564	940.907	-164.840
300	442.281	665.033	662.314	0.815	690.305	942.458	-164.093
350	519.692	739.087	667.986	24.885	683.871	985.008	-147.001
400	591.272	813.228	681.511	52.687	678.335	1028.404	-134.293
450	656.028	886.677	700.236	83.898	673.584	1072.454	-124.485
500	713.887	958.850	722.501	118.174	669.508	1117.022	-116.692
600	810.944	1097.936	773.590	194.608	663.000	1207.173	-105.092
700	887.787	1228.939	829.381	279.690	658.420	1298.264	-96.876
800	949.497	1351.660	887.081	371.663	655.549	1389.872	-90.747
900	999.844	1466.498	945.151	469.212	654.168	1481.742	-85.996
1000	1041.471	1574.064	1002.722	571.342	654.076	1573.710	-82.200
1100	1076.253	1675.006	1059.298	677.279	655.027	1665.647	-79.093
1200	1105.561	1769.944	1114.603	786.410	656.844	1757.436	-76.498
1300	1130.432	1859.445	1168.489	898.243	659.301	1849.059	-74.295
1400	1151.669	1944.017	1220.891	1012.376	662.234	1940.480	-72.399
1500	1169.906	2024.111	1271.793	1128.477	665.539	2031.680	-70.748
1600	1185.650	2100.130	1321.209	1246.274	669.056	2122.640	-69.296
1700	1199.311	2172.429	1369.172	1365.538	672.692	2213.345	-68.006
1800	1211.222	2241.325	1415.726	1486.078	676.354	2303.916	-66.857
1900	1221.654	2307.098	1460.923	1607.733	680.003	2394.217	-65.820
2000	1230.833	2369.999	1504.815	1730.367	683.571	2484.361	-64.884
2100	1238.942	2430.251	1547.459	1853.864	686.962	2574.313	-64.031
2200	1246.134	2488.056	1588.909	1978.125	690.175	2664.111	-63.253
2300	1252.539	2543.593	1629.217	2103.064	693.202	2753.765	-62.539
2400	1258.263	2597.024	1668.437	2228.610	695.958	2843.233	-61.880
2500	1263.396	2648.495	1706.616	2354.697	698.455	2932.733	-61.275
2600	1268.015	2698.138	1743.802	2481.272	700.650	3021.993	-60.711
2700	1272.184	2746.072	1780.041	2608.285	702.547	3111.265	-60.190
2800	1275.958	2792.408	1815.374	2735.695	704.115	3200.500	-59.705
2900	1279.384	2837.244	1849.842	2863.465	705.317	3289.618	-59.251
3000	1282.503	2880.670	1883.483	2991.562	706.208	3378.733	-58.828
3100	1285.350	2922.770	1916.333	3119.957	706.691	3467.729	-58.430
3200	1287.955	2963.620	1948.425	3248.624	706.818	3556.807	-58.058
3300	1290.344	3003.290	1979.793	3377.541	706.567	3645.936	-57.709
3400	1292.540	3041.844	2010.465	3506.687	705.902	3734.970	-57.380
3500	1294.563	3079.341	2040.471	3636.043	704.831	3824.007	-57.069
3600	1296.430	3115.836	2069.838	3765.594	703.380	3913.189	-56.778
3700	1298.156	3151.381	2098.591	3895.324	701.510	4002.439	-56.503
3800	1299.756	3186.022	2126.753	4025.221	699.189	4091.669	-56.243
3900	1301.241	3219.803	2154.349	4155.272	696.468	4180.902	-55.996
4000	1302.621	3252.765	2181.399	4285.466	693.325	4270.384	-55.764
4100	1303.907	3284.947	2207.924	4415.793	689.719	4359.856	-55.544
4200	1305.106	3316.382	2233.943	4546.244	685.682	4449.411	-55.335
4300	1306.226	3347.105	2259.475	4676.811	681.197	4538.954	-55.136
4400	1307.274	3377.147	2284.536	4807.487	676.277	4628.723	-54.949
4500	1308.256	3406.536	2309.144	4938.264	670.938	4718.678	-54.772
4600	1309.177	3435.300	2333.314	5069.136	665.116	4808.767	-54.604
4700	1310.041	3463.465	2357.061	5200.097	658.829	4898.844	-54.443
4800	1310.855	3491.055	2380.400	5331.143	652.137	4989.193	-54.292
4900	1311.621	3518.091	2403.343	5462.267	644.945	5079.516	-54.147
5000	1312.342	3544.597	2425.904	5593.465	637.371	5170.226	-54.012

3.618. Dinaphtho[8,1,2-*abc*:2',1',8'-*nop*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128395-02-8
Point Group: C₂

Length: 14.16 Å
Width: 13.62 Å
Breadth: 5.014 Å
L/B Ratio: 1.040

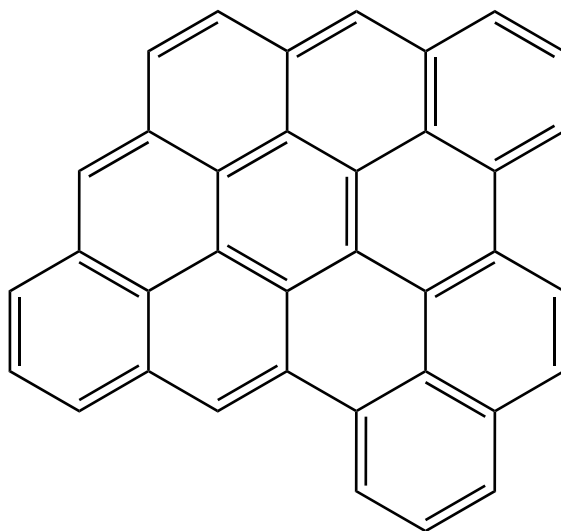
Cartesian coordinates:

C	5.0677	-0.9444	0.0694	C	1.9790	4.3500	0.2263	H	2.8691	4.9824	0.3238
C	3.9316	-1.8126	-0.1343	C	0.7404	4.9045	0.1210	H	0.6101	5.9927	0.1286
C	2.6214	-1.2776	-0.0569	C	-0.4187	4.0802	-0.0001	H	-3.8212	4.2959	-0.3239
C	2.4565	0.1356	0.0941	C	-2.7036	2.4322	-0.2058	H	-1.8145	5.7439	-0.1288
C	3.5955	0.9828	0.2188	C	-2.8213	3.8574	-0.2264	H	-4.8346	2.0698	-0.3838
C	4.9093	0.3834	0.2453	C	-1.7210	4.6519	-0.1211	H	4.3135	3.0085	0.3837
C	1.4905	-2.1216	-0.1861	C	-2.4328	-0.3661	-0.0941	H	-0.0226	-4.2149	0.7706
C	1.7252	-3.4561	-0.5576	C	-3.7201	0.2321	-0.2188	H	-2.0668	-5.5495	0.9577
C	3.0074	-3.9664	-0.6722	C	-3.8442	1.6086	-0.2845	H	-4.2920	-4.5469	0.4851
C	4.1151	-3.1619	-0.4268	C	3.4374	2.3558	0.2845	H	-5.6538	-2.6029	-0.0718
C	1.1693	0.6873	0.0555	C	-2.3073	-1.7834	0.0569	H	-5.8628	-0.1512	-0.3989
C	0.0183	-0.1784	0.0000	C	-1.0285	-2.3801	0.1862	H	5.1260	-3.5805	-0.4850
C	0.1605	-1.5645	0.0000	C	-3.4815	-2.5733	0.1344	H	3.1508	-5.0141	-0.9575
C	-1.2845	0.4355	-0.0555	C	-3.3872	-3.9317	0.4269	H	0.8781	-4.1225	-0.7705
C	-1.4261	1.8467	-0.0917	C	-2.1392	-4.4945	0.6723	H	5.7714	1.0426	0.3988
C	-0.2760	2.6900	-0.0000	C	-0.9874	-3.7344	0.5577	H	6.0646	-1.4004	0.0719
C	1.0214	2.0978	0.0917	C	-4.8848	-0.6217	-0.2453				
C	2.1533	2.9307	0.2057	C	-4.7703	-1.9539	-0.0694				

Table 3.618: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*abc*:2',1',8'-*nop*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.113	528.305	528.305	∞
100	119.435	353.813	876.029	-52.222	555.503	604.131	-315.559
200	262.034	478.230	645.511	-33.456	540.980	658.584	-172.001
250	342.359	545.291	618.711	-18.355	534.258	688.761	-143.906
298.15	419.757	612.235	612.235	0.000	528.305	719.074	-125.976
300	422.686	614.840	612.243	0.779	528.084	720.255	-125.405
350	499.565	685.832	617.674	23.855	522.612	752.730	-112.336
400	570.780	757.260	630.658	50.641	517.869	785.924	-102.629
450	635.297	828.281	648.678	80.821	513.754	819.683	-95.144
500	692.963	898.259	670.148	114.056	510.165	853.899	-89.204
600	789.501	1033.490	719.533	188.374	504.243	923.231	-80.373
700	865.437	1161.124	773.596	271.270	499.806	993.441	-74.130
800	925.841	1280.779	829.598	360.945	496.702	1064.175	-69.482
900	974.603	1392.741	886.018	456.051	494.756	1135.216	-65.885
1000	1014.505	1497.559	941.988	555.571	493.816	1206.436	-63.016
1100	1047.536	1595.849	997.009	658.724	493.672	1277.725	-60.673
1200	1075.142	1688.215	1050.801	764.898	494.186	1348.971	-58.718
1300	1098.405	1775.217	1103.211	873.608	495.164	1420.170	-57.062
1400	1118.152	1857.360	1154.173	984.462	496.466	1491.284	-55.639
1500	1135.026	1935.095	1203.667	1097.142	498.019	1562.301	-54.403
1600	1149.531	2008.822	1251.705	1211.388	499.677	1633.196	-53.317
1700	1162.073	2078.898	1298.319	1326.983	501.368	1703.959	-52.355
1800	1172.974	2145.636	1343.553	1443.748	503.009	1774.702	-51.499
1900	1182.498	2209.316	1387.457	1561.532	504.573	1845.289	-50.729
2000	1190.858	2270.187	1430.083	1680.209	506.006	1915.831	-50.035
2100	1198.229	2328.471	1471.485	1799.671	507.216	1986.289	-49.405
2200	1204.756	2384.367	1511.718	1919.827	508.207	2056.693	-48.831
2300	1210.559	2438.051	1550.834	2040.598	508.983	2127.063	-48.306
2400	1215.739	2489.683	1588.884	2161.918	509.454	2197.338	-47.823
2500	1220.379	2539.408	1625.917	2283.728	509.644	2267.745	-47.381
2600	1224.549	2587.355	1661.979	2405.978	509.511	2338.000	-46.970
2700	1228.310	2633.641	1697.114	2528.624	509.061	2408.367	-46.592
2800	1231.712	2678.375	1731.365	2651.628	508.265	2478.774	-46.241
2900	1234.798	2721.652	1764.770	2774.956	507.089	2549.154	-45.914
3000	1237.606	2763.561	1797.369	2898.578	505.591	2619.615	-45.611
3100	1240.167	2804.185	1829.195	3022.469	503.674	2690.027	-45.326
3200	1242.509	2843.596	1860.282	3146.604	501.393	2760.607	-45.061
3300	1244.656	2881.863	1890.662	3270.964	498.729	2831.317	-44.815
3400	1246.628	2919.050	1920.364	3395.530	495.642	2901.994	-44.583
3500	1248.444	2955.213	1949.417	3520.285	492.145	2972.747	-44.365
3600	1250.120	2990.406	1977.847	3645.214	488.267	3043.725	-44.162
3700	1251.669	3024.680	2005.679	3770.304	483.965	3114.829	-43.973
3800	1253.104	3058.079	2032.936	3895.544	479.213	3185.987	-43.794
3900	1254.435	3090.646	2059.641	4020.922	474.058	3257.199	-43.624
4000	1255.672	3122.422	2085.815	4146.428	468.484	3328.734	-43.468
4100	1256.824	3153.442	2111.478	4272.053	462.446	3400.318	-43.320
4200	1257.899	3183.741	2136.648	4397.790	455.979	3472.044	-43.180
4300	1258.902	3213.352	2161.345	4523.631	449.067	3543.812	-43.048
4400	1259.840	3242.304	2185.584	4649.568	441.721	3615.861	-42.925
4500	1260.719	3270.627	2209.383	4775.597	433.961	3688.152	-42.810
4600	1261.544	3298.345	2232.756	4901.710	425.719	3760.641	-42.703
4700	1262.318	3325.484	2255.718	5027.904	417.016	3833.163	-42.600
4800	1263.046	3352.068	2278.282	5154.172	407.909	3906.014	-42.505
4900	1263.731	3378.118	2300.463	5280.512	398.304	3978.879	-42.414
5000	1264.377	3403.656	2322.272	5406.917	388.322	4052.183	-42.332

3.619. Dibenzo[*ef,no*]naphtho[8,1,2-*abc*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128515-16-2
Point Group: C_s

Length: 15.85 Å
Width: 14.14 Å
Breadth: 3.892 Å
L/B Ratio: 1.121

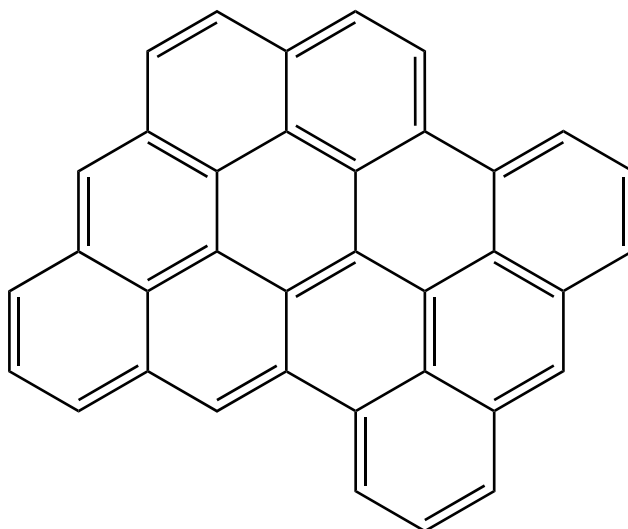
Cartesian coordinates:

C	2.4526	-3.9352	0.0000	C	-4.7551	-2.8160	0.0000	H	3.3200	-4.6057	0.0000
C	1.1991	-4.4241	0.0000	C	-3.6724	-3.6769	0.0000	H	1.0148	-5.5048	0.0000
C	2.7114	-2.5067	0.0000	C	-3.2791	-0.8933	0.0000	H	4.8494	-2.6854	0.0000
C	3.9849	-2.0101	0.0000	C	-2.1631	-1.7666	0.0000	H	6.3818	-0.7589	0.0000
C	4.2237	-0.5977	0.0000	C	-0.8316	-1.2417	0.0000	H	6.7500	1.6934	0.0000
C	5.5255	-0.0750	0.0000	C	-0.6185	0.1580	0.0000	H	4.8279	3.2598	0.0000
C	5.7291	1.2966	0.0000	C	0.6854	0.6700	0.0000	H	-1.4114	-5.1262	0.0000
C	4.6514	2.1783	0.0000	C	0.9312	2.0949	0.0000	H	2.3886	3.6585	0.0000
C	0.0413	-3.5484	0.0000	C	-0.2177	2.9990	0.0000	H	-5.4294	-0.7559	0.0000
C	-1.2320	-4.0438	0.0000	C	-0.0470	4.3712	0.0000	H	-5.7738	-3.2182	0.0000
C	0.2670	-2.1252	0.0000	C	-1.1539	5.2381	0.0000	H	-3.8282	-4.7616	0.0000
C	1.5796	-1.6140	0.0000	C	-2.4303	4.7342	0.0000	H	0.9730	4.7860	0.0000
C	1.7894	-0.2200	0.0000	C	-1.5363	2.4595	0.0000	H	-0.9839	6.3198	0.0000
C	3.1233	0.2908	0.0000	C	-2.6419	3.3339	0.0000	H	-3.2975	5.4042	0.0000
C	3.3431	1.6894	0.0000	C	-3.9599	2.7932	0.0000	H	-4.8121	3.4824	0.0000
C	2.2101	2.5708	0.0000	C	-4.1548	1.4440	0.0000	H	-5.1703	1.0185	0.0000
C	-2.3637	-3.1659	0.0000	C	-3.0538	0.5417	0.0000				
C	-4.5632	-1.4353	0.0000	C	-1.7571	1.0468	0.0000				

Table 3.619: Table of thermodynamic data as a function of temperature for Dibenzo[*ef,no*]naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.908	537.328	537.328	∞
100	123.033	370.425	896.967	-52.654	564.094	611.060	-319.178
200	264.104	496.920	664.911	-33.598	549.862	663.727	-173.344
250	343.759	564.367	638.012	-18.411	543.225	692.959	-144.783
298.15	420.721	631.517	631.517	0.000	537.328	722.349	-126.550
300	423.636	634.129	631.525	0.781	537.109	723.494	-125.969
350	500.223	705.244	636.967	23.897	531.677	755.001	-112.675
400	571.249	776.746	649.971	50.710	526.962	787.222	-102.799
450	635.640	847.814	668.012	80.911	522.867	820.006	-95.182
500	693.219	917.824	689.504	114.160	519.292	853.244	-89.136
600	789.650	1053.091	738.928	188.498	513.390	920.618	-80.145
700	865.524	1180.743	793.021	271.405	508.965	988.866	-73.789
800	925.889	1300.407	849.048	361.087	505.867	1057.638	-69.055
900	974.624	1412.373	905.488	456.197	503.925	1126.716	-65.392
1000	1014.509	1517.192	961.475	555.718	502.986	1195.973	-62.470
1100	1047.528	1615.482	1016.509	658.870	502.842	1265.298	-60.083
1200	1075.126	1707.847	1070.311	765.043	503.355	1334.582	-58.092
1300	1098.384	1794.848	1122.731	873.751	504.331	1403.817	-56.405
1400	1118.128	1876.989	1173.701	984.603	505.631	1472.968	-54.956
1500	1135.000	1954.722	1223.201	1097.281	507.181	1542.022	-53.697
1600	1149.505	2028.448	1271.245	1211.524	508.836	1610.955	-52.591
1700	1162.047	2098.521	1317.864	1327.117	510.525	1679.755	-51.612
1800	1172.948	2165.258	1363.103	1443.879	512.163	1748.536	-50.740
1900	1182.473	2228.937	1407.010	1561.661	513.725	1817.161	-49.956
2000	1190.833	2289.807	1449.639	1680.335	515.155	1885.741	-49.249
2100	1198.205	2348.090	1491.045	1799.794	516.362	1954.237	-48.608
2200	1204.733	2403.984	1531.281	1919.948	517.352	2022.680	-48.024
2300	1210.538	2457.667	1570.399	2040.717	518.125	2091.088	-47.489
2400	1215.718	2509.299	1608.451	2162.035	518.594	2159.401	-46.997
2500	1220.359	2559.022	1645.485	2283.843	518.782	2227.846	-46.547
2600	1224.531	2606.969	1681.549	2406.091	518.647	2296.140	-46.129
2700	1228.292	2653.254	1716.686	2528.735	518.195	2364.545	-45.744
2800	1231.695	2697.987	1750.938	2651.737	517.397	2432.992	-45.387
2900	1234.782	2741.264	1784.345	2775.064	516.219	2501.410	-45.054
3000	1237.591	2783.173	1816.945	2898.684	514.720	2569.910	-44.745
3100	1240.152	2823.795	1848.772	3022.573	512.801	2638.361	-44.455
3200	1242.495	2863.206	1879.860	3146.708	510.519	2706.979	-44.186
3300	1244.642	2901.473	1910.241	3271.066	507.854	2775.729	-43.935
3400	1246.615	2938.659	1939.944	3395.630	504.766	2844.445	-43.699
3500	1248.432	2974.822	1968.998	3520.384	501.268	2913.236	-43.477
3600	1250.108	3010.015	1997.429	3645.312	497.388	2982.254	-43.270
3700	1251.658	3044.288	2025.261	3770.401	493.085	3051.397	-43.077
3800	1253.093	3077.687	2052.519	3895.640	488.332	3120.595	-42.895
3900	1254.425	3110.254	2079.225	4021.016	483.176	3189.845	-42.722
4000	1255.662	3142.029	2105.399	4146.521	477.601	3259.420	-42.563
4100	1256.815	3173.049	2131.063	4272.146	471.562	3329.043	-42.412
4200	1257.890	3203.349	2156.234	4397.882	465.094	3398.808	-42.269
4300	1258.893	3232.959	2180.931	4523.722	458.181	3468.615	-42.134
4400	1259.832	3261.911	2205.171	4649.658	450.834	3538.704	-42.009
4500	1260.711	3290.233	2228.970	4775.686	443.074	3609.034	-41.892
4600	1261.536	3317.952	2252.343	4901.799	434.831	3679.562	-41.782
4700	1262.311	3345.091	2275.305	5027.992	426.127	3750.123	-41.677
4800	1263.039	3371.674	2297.870	5154.259	417.019	3821.014	-41.580
4900	1263.724	3397.725	2320.052	5280.598	407.414	3891.919	-41.488
5000	1264.370	3423.262	2341.861	5407.003	397.431	3963.262	-41.403

3.620. Anthra[1,9,8-*abcd*]benzo[*hi*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128345-78-8
Point Group: C_s

Length: 14.76 Å
Width: 12.73 Å
Breadth: 3.889 Å
L/B Ratio: 1.160

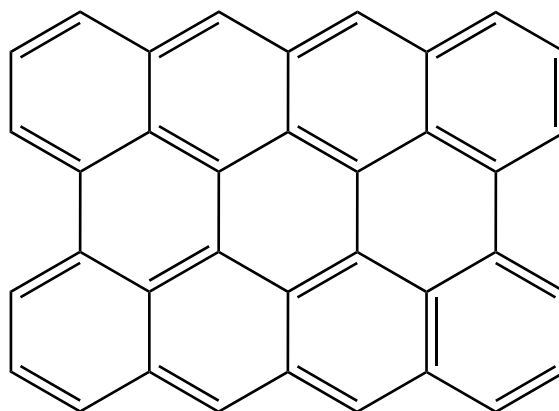
Cartesian coordinates:

C	-0.2380	-4.3805	0.0000	C	-5.3450	-1.8362	0.0000	H	-0.1749	-5.4746	0.0000
C	-1.4875	-3.7612	0.0000	C	-4.0783	-2.4696	0.0000	H	-2.4036	-4.3726	0.0000
C	-1.6069	-2.3752	0.0000	C	-0.7357	2.7137	0.0000	H	2.2793	-5.3274	0.0000
C	-0.4378	-1.5746	0.0000	C	-0.8638	4.0813	0.0000	H	4.3454	-3.9587	0.0000
C	0.8292	-2.2013	0.0000	C	-2.1414	4.6970	0.0000	H	5.4321	-1.7566	0.0000
C	0.9232	-3.6176	0.0000	C	-3.2739	3.9412	0.0000	H	1.6658	3.9101	0.0000
C	2.2315	-4.2322	0.0000	C	-1.8200	0.4877	0.0000	H	-6.4160	0.0215	0.0000
C	3.3557	-3.4873	0.0000	C	-1.9127	1.8912	0.0000	H	-6.2452	-2.4597	0.0000
C	2.0137	-1.4092	0.0000	C	-3.1915	2.5121	0.0000	H	-4.0225	-3.5692	0.0000
C	3.3005	-2.0408	0.0000	C	-4.3460	1.7273	0.0000	H	0.0397	4.7107	0.0000
C	4.4449	-1.2783	0.0000	C	-4.2600	0.3310	0.0000	H	-2.1974	5.7906	0.0000
C	1.9194	-0.0110	0.0000	C	-2.9874	-0.2996	0.0000	H	-4.2653	4.4083	0.0000
C	1.7235	2.8093	0.0000	C	3.1076	0.7736	0.0000	H	-5.3314	2.2097	0.0000
C	0.6361	0.6237	0.0000	C	4.3718	0.1424	0.0000	H	6.5185	0.4528	0.0000
C	0.5778	2.0727	0.0000	C	5.5371	0.9404	0.0000	H	6.3478	2.9279	0.0000
C	-0.5177	-0.1461	0.0000	C	5.4400	2.3152	0.0000	H	4.1341	4.0416	0.0000
C	-2.9176	-1.7332	0.0000	C	4.1894	2.9472	0.0000				
C	-5.4396	-0.4763	0.0000	C	3.0242	2.1923	0.0000				

Table 3.620: Table of thermodynamic data as a function of temperature for Anthra[1,9,8-*abcd*]benzo[*hi*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.739	571.903	571.903	∞
100	122.528	368.830	894.190	-52.536	598.787	645.913	-337.383
200	263.480	494.926	662.617	-33.538	584.497	698.761	-182.494
250	343.144	562.234	635.763	-18.382	577.829	728.096	-152.124
298.15	420.142	629.279	629.279	0.000	571.903	757.591	-132.724
300	423.059	631.887	629.287	0.780	571.683	758.741	-132.106
350	499.700	702.917	634.721	23.868	566.223	790.362	-117.953
400	570.785	774.353	647.711	50.657	561.484	822.701	-107.432
450	635.235	845.370	665.735	80.836	557.367	855.606	-99.314
500	692.867	915.340	687.208	114.066	553.773	888.967	-92.868
600	789.386	1050.551	736.595	188.373	547.840	956.592	-83.277
700	865.323	1178.167	790.656	271.258	543.393	1025.097	-76.492
800	925.733	1297.807	846.655	360.922	540.277	1094.127	-71.438
900	974.500	1409.757	903.071	456.017	538.320	1163.467	-67.524
1000	1014.409	1514.565	959.037	555.527	537.370	1232.986	-64.403
1100	1047.444	1612.846	1014.054	658.671	537.218	1302.574	-61.853
1200	1075.056	1705.204	1067.841	764.836	537.723	1372.121	-59.726
1300	1098.324	1792.199	1120.247	873.537	538.692	1441.621	-57.924
1400	1118.077	1874.336	1171.205	984.384	539.987	1511.038	-56.376
1500	1134.955	1952.066	1220.695	1097.057	541.532	1580.357	-55.032
1600	1149.465	2025.789	1268.729	1211.296	543.183	1649.556	-53.851
1700	1162.011	2095.860	1315.340	1326.885	544.868	1718.622	-52.806
1800	1172.917	2162.595	1360.571	1443.644	546.503	1787.669	-51.876
1900	1182.444	2226.272	1404.471	1561.422	548.061	1856.560	-51.039
2000	1190.807	2287.141	1447.094	1680.094	549.489	1925.407	-50.285
2100	1198.182	2345.423	1488.494	1799.551	550.694	1994.169	-49.601
2200	1204.712	2401.316	1528.724	1919.702	551.681	2062.878	-48.978
2300	1210.518	2454.998	1567.838	2040.469	552.452	2131.553	-48.408
2400	1215.700	2506.629	1605.885	2161.785	552.920	2200.134	-47.884
2500	1220.343	2556.352	1642.916	2283.591	553.106	2268.846	-47.404
2600	1224.515	2604.297	1678.975	2405.838	552.969	2337.407	-46.958
2700	1228.278	2650.583	1714.109	2528.480	552.515	2406.080	-46.547
2800	1231.682	2695.315	1748.357	2651.481	551.716	2474.793	-46.167
2900	1234.770	2738.591	1781.761	2774.806	550.537	2543.478	-45.812
3000	1237.579	2780.500	1814.358	2898.426	549.037	2612.246	-45.482
3100	1240.141	2821.122	1846.182	3022.314	547.117	2680.964	-45.173
3200	1242.485	2860.532	1877.268	3146.447	544.834	2749.850	-44.886
3300	1244.633	2898.799	1907.646	3270.804	542.167	2818.866	-44.618
3400	1246.606	2935.985	1937.347	3395.367	539.078	2887.850	-44.365
3500	1248.423	2972.147	1966.399	3520.120	535.579	2956.909	-44.129
3600	1250.100	3007.340	1994.827	3645.048	531.699	3026.194	-43.908
3700	1251.650	3041.613	2022.658	3770.136	527.395	3095.605	-43.701
3800	1253.086	3075.012	2049.914	3895.374	522.641	3165.070	-43.506
3900	1254.418	3107.579	2076.617	4020.750	517.485	3234.588	-43.322
4000	1255.656	3139.354	2102.790	4146.254	511.909	3304.430	-43.151
4100	1256.809	3170.374	2128.452	4271.878	505.869	3374.321	-42.988
4200	1257.884	3200.673	2153.622	4397.613	499.400	3444.354	-42.836
4300	1258.888	3230.283	2178.317	4523.452	492.487	3514.428	-42.691
4400	1259.827	3259.235	2202.556	4649.389	485.140	3584.785	-42.556
4500	1260.706	3287.557	2226.354	4775.416	477.379	3655.382	-42.430
4600	1261.531	3315.275	2249.726	4901.528	469.135	3726.178	-42.311
4700	1262.306	3342.414	2272.687	5027.720	460.431	3797.007	-42.198
4800	1263.034	3368.998	2295.250	5153.988	451.323	3868.165	-42.093
4900	1263.720	3395.048	2317.430	5280.326	441.717	3939.338	-41.993
5000	1264.366	3420.585	2339.239	5406.730	431.733	4010.949	-41.901

3.621. Tetrabenzo[bc,ef,kl,no]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128345-80-2
Point Group: D_{2h}

Length: 14.07 Å
Width: 11.71 Å
Breadth: 3.885 Å
L/B Ratio: 1.202

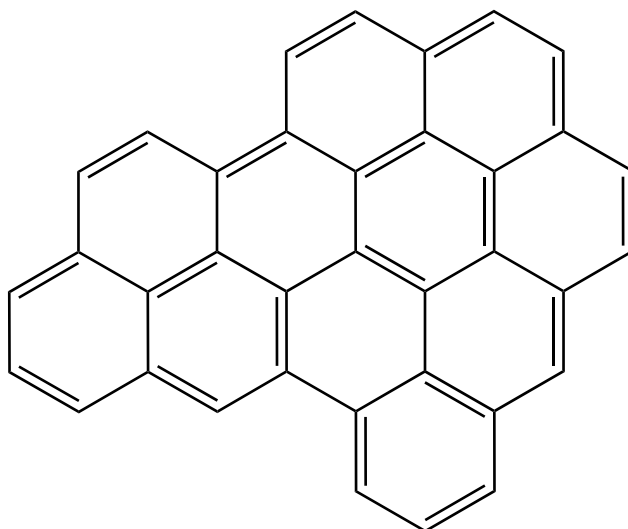
Cartesian coordinates:

C	-4.8649	-1.4719	0.0000	C	-3.7067	0.7109	0.0000	H	-5.8304	-0.9426	0.0000
C	-4.8461	-2.8931	0.0000	C	-3.7049	3.5329	0.0000	H	-5.8013	-3.4284	0.0000
C	-3.6679	-3.5713	0.0000	C	-4.8760	2.8424	0.0000	H	-3.6459	-4.6670	0.0000
C	-2.4190	-2.8641	0.0000	C	-4.8800	1.4211	0.0000	H	-1.2000	-4.6430	0.0000
C	-1.2098	-3.5459	0.0000	C	-2.4488	2.8387	0.0000	H	1.2483	-4.6302	0.0000
C	0.0148	-2.8470	0.0000	C	-2.4503	1.4115	0.0000	H	3.6943	-4.6288	0.0000
C	1.2467	-3.5331	0.0000	C	-1.2358	0.7165	0.0000	H	5.8368	-3.3677	0.0000
C	2.4488	-2.8387	0.0000	C	-1.2467	3.5331	0.0000	H	5.8398	-0.8817	0.0000
C	3.7049	-3.5329	0.0000	C	-0.0148	2.8470	0.0000	H	-3.6943	4.6288	0.0000
C	4.8760	-2.8424	0.0000	C	-0.0074	1.4231	0.0000	H	-5.8368	3.3677	0.0000
C	4.8800	-1.4211	0.0000	C	1.2283	0.7293	0.0000	H	-5.8399	0.8818	0.0000
C	-3.6990	-0.7495	0.0000	C	1.2098	3.5459	0.0000	H	-1.2483	4.6302	0.0000
C	-2.4354	-1.4370	0.0000	C	2.4191	2.8641	0.0000	H	1.2000	4.6430	0.0000
C	-1.2283	-0.7293	0.0000	C	2.4354	1.4370	0.0000	H	5.8303	0.9426	0.0000
C	0.0074	-1.4231	0.0000	C	3.6990	0.7495	0.0000	H	5.8014	3.4283	0.0000
C	1.2358	-0.7165	0.0000	C	4.8649	1.4719	0.0000	H	3.6459	4.6670	0.0000
C	2.4503	-1.4115	0.0000	C	4.8461	2.8930	0.0000				
C	3.7066	-0.7109	0.0000	C	3.6679	3.5713	0.0000				

Table 3.621: Table of thermodynamic data as a function of temperature for Tetra-benzo[bc,ef,kl,no]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-59.827	624.638	624.638	∞
100	122.573	354.224	881.183	-52.696	651.362	699.949	-365.608
200	264.369	480.673	648.885	-33.642	637.128	754.243	-196.984
250	344.216	548.200	621.949	-18.437	630.509	784.285	-163.864
298.15	421.343	615.445	615.445	0.000	624.638	814.451	-142.685
300	424.264	618.061	615.453	0.782	624.420	815.626	-142.010
350	500.997	689.284	620.903	23.933	619.023	847.933	-126.545
400	572.131	760.897	633.927	50.788	614.350	880.950	-115.038
450	636.590	832.073	651.996	81.035	610.301	914.524	-106.153
500	694.203	902.185	673.520	114.332	606.775	948.546	-99.092
600	790.623	1037.632	723.017	188.769	600.971	1017.474	-88.577
700	866.429	1165.429	777.186	271.770	596.640	1087.261	-81.131
800	926.705	1285.208	833.285	361.538	593.628	1157.558	-75.579
900	975.350	1397.265	889.793	456.725	591.763	1228.152	-71.279
1000	1015.151	1502.157	945.842	556.314	590.893	1298.916	-67.847
1100	1048.095	1600.504	1000.934	659.527	590.809	1369.741	-65.042
1200	1075.628	1692.916	1054.788	765.753	591.376	1440.520	-62.703
1300	1098.831	1779.954	1107.255	874.509	592.399	1511.247	-60.721
1400	1118.527	1862.126	1158.267	985.403	593.741	1581.886	-59.020
1500	1135.357	1939.886	1207.806	1098.119	595.329	1652.425	-57.541
1600	1149.826	2013.633	1255.886	1212.396	597.018	1722.840	-56.244
1700	1162.336	2083.725	1302.538	1328.019	598.737	1793.121	-55.095
1800	1173.211	2150.478	1347.806	1444.808	600.403	1863.381	-54.073
1900	1182.712	2214.170	1391.741	1562.615	601.989	1933.483	-53.154
2000	1191.051	2275.052	1434.396	1681.312	603.442	2003.539	-52.326
2100	1198.405	2333.345	1475.825	1800.793	604.671	2073.509	-51.575
2200	1204.917	2389.248	1516.082	1920.965	605.679	2143.426	-50.890
2300	1210.707	2442.939	1555.221	2041.752	606.470	2213.307	-50.265
2400	1215.875	2494.578	1593.292	2163.086	606.956	2283.093	-49.689
2500	1220.505	2544.308	1630.344	2284.909	607.159	2353.010	-49.162
2600	1224.666	2592.259	1666.424	2407.171	607.037	2422.776	-48.673
2700	1228.418	2638.550	1701.576	2529.829	606.599	2492.651	-48.222
2800	1231.813	2683.287	1735.843	2652.843	605.813	2562.568	-47.804
2900	1234.892	2726.568	1769.264	2776.181	604.647	2632.456	-47.415
3000	1237.694	2768.480	1801.876	2899.812	603.158	2702.425	-47.052
3100	1240.249	2809.106	1833.716	3023.711	601.249	2772.346	-46.713
3200	1242.586	2848.520	1864.815	3147.855	598.977	2842.433	-46.397
3300	1244.729	2886.790	1895.207	3272.222	596.320	2912.650	-46.102
3400	1246.697	2923.978	1924.921	3396.795	593.241	2982.835	-45.825
3500	1248.509	2960.143	1953.985	3521.556	589.750	3053.094	-45.564
3600	1250.181	2995.339	1982.424	3646.492	585.878	3123.580	-45.321
3700	1251.727	3029.614	2010.266	3771.588	581.582	3194.190	-45.093
3800	1253.159	3063.014	2037.532	3896.833	576.835	3264.855	-44.878
3900	1254.487	3095.583	2064.246	4022.216	571.687	3335.573	-44.674
4000	1255.722	3127.360	2090.428	4147.728	566.118	3406.614	-44.485
4100	1256.872	3158.381	2116.099	4273.358	560.084	3477.705	-44.306
4200	1257.944	3188.682	2141.277	4399.099	553.622	3548.937	-44.137
4300	1258.945	3218.294	2165.981	4524.944	546.715	3620.210	-43.976
4400	1259.882	3247.247	2190.227	4650.886	539.372	3691.765	-43.826
4500	1260.759	3275.570	2214.033	4776.919	531.617	3763.561	-43.685
4600	1261.581	3303.289	2237.412	4903.036	523.378	3835.556	-43.553
4700	1262.354	3330.429	2260.380	5029.233	514.679	3907.584	-43.427
4800	1263.080	3357.014	2282.950	5155.505	505.576	3979.940	-43.310
4900	1263.764	3383.065	2305.137	5281.848	495.974	4052.311	-43.197
5000	1264.409	3408.603	2326.952	5408.257	485.995	4125.120	-43.094

3.622. Benzo[*ef*]phenaleno[9,1,2-*abc*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128345-76-6
Point Group: C_s

Length: 15.88 Å
Width: 12.90 Å
Breadth: 3.889 Å
L/B Ratio: 1.231

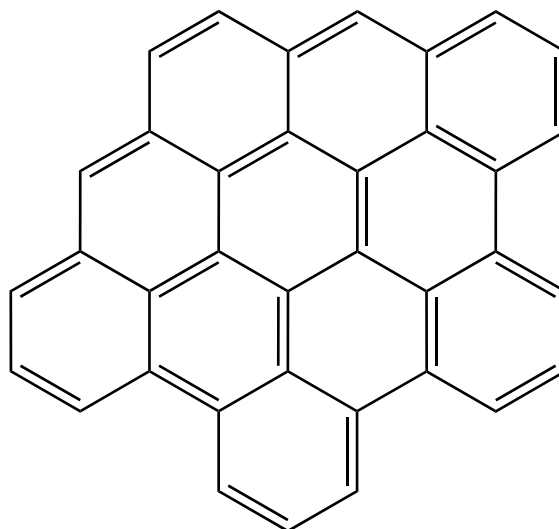
Cartesian coordinates:

C	5.3276	-0.2036	0.0000	C	-1.1331	0.3132	0.0000	H	6.3754	-0.5255	0.0000
C	5.0028	1.1092	0.0000	C	0.2127	-0.0686	0.0000	H	5.7801	1.8821	0.0000
C	3.6255	1.5388	0.0000	C	0.5611	-1.4423	0.0000	H	4.0736	3.6474	0.0000
C	3.2875	2.8821	0.0000	C	-0.4401	-2.4351	0.0000	H	2.3831	5.4125	0.0000
C	1.9357	3.2831	0.0000	C	-0.0457	-3.8151	0.0000	H	-0.0064	6.0995	0.0000
C	1.5834	4.6632	0.0000	C	1.2609	-4.1793	0.0000	H	-1.8094	4.3888	0.0000
C	0.2694	5.0397	0.0000	C	2.2972	-3.1891	0.0000	H	3.9279	-4.6167	0.0000
C	-0.7560	4.0685	0.0000	C	1.9418	-1.8296	0.0000	H	5.7017	-2.8807	0.0000
C	4.3084	-1.2207	0.0000	C	-3.8729	1.0763	0.0000	H	-3.1113	3.1282	0.0000
C	3.6619	-3.5534	0.0000	C	-5.2215	1.4430	0.0000	H	-0.8459	-4.5712	0.0000
C	4.6444	-2.5918	0.0000	C	-6.2133	0.4676	0.0000	H	1.5507	-5.2363	0.0000
C	2.9595	-0.8391	0.0000	C	-5.8819	-0.8800	0.0000	H	-5.4957	2.5040	0.0000
C	2.5998	0.5512	0.0000	C	-3.5226	-0.2946	0.0000	H	-7.2666	0.7676	0.0000
C	1.2539	0.9336	0.0000	C	-4.5387	-1.2761	0.0000	H	-6.6702	-1.6413	0.0000
C	0.9100	2.3079	0.0000	C	-4.1631	-2.6632	0.0000	H	-4.9597	-3.4160	0.0000
C	-0.4583	2.7231	0.0000	C	-2.8590	-3.0278	0.0000	H	-2.5655	-4.0890	0.0000
C	-1.5124	1.7097	0.0000	C	-1.8041	-2.0513	0.0000				
C	-2.8301	2.0623	0.0000	C	-2.1438	-0.6834	0.0000				

Table 3.622: Table of thermodynamic data as a function of temperature for Benzo[*ef*]phenaleno[9,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.330	525.597	525.597	∞
100	121.065	364.761	887.368	-52.261	552.756	600.289	-313.552
200	262.073	489.797	656.874	-33.415	538.313	653.604	-170.700
250	341.907	556.810	630.112	-18.325	531.579	683.203	-142.744
298.15	419.008	623.646	623.646	0.000	525.597	712.964	-124.906
300	421.928	626.247	623.655	0.778	525.375	714.124	-124.337
350	498.632	697.108	629.076	23.811	519.860	746.032	-111.337
400	569.761	768.404	642.036	50.547	515.068	778.665	-101.681
450	634.252	839.303	660.023	80.676	510.901	811.870	-94.238
500	691.928	909.172	681.455	113.859	507.260	845.537	-88.331
600	788.544	1044.220	730.759	188.077	501.238	913.788	-79.551
700	864.581	1171.714	784.740	270.882	496.711	982.932	-73.346
800	925.084	1291.261	840.666	360.477	493.525	1052.612	-68.727
900	973.934	1403.140	897.016	455.512	491.508	1122.610	-65.153
1000	1013.914	1507.892	952.923	554.969	490.505	1192.794	-62.304
1100	1047.011	1606.128	1007.887	658.065	490.306	1263.052	-59.976
1200	1074.674	1698.451	1061.626	764.190	490.771	1333.272	-58.035
1300	1097.986	1785.418	1113.990	872.855	491.704	1403.449	-56.390
1400	1117.775	1867.531	1164.910	983.670	492.967	1473.545	-54.978
1500	1134.686	1945.241	1214.365	1096.315	494.483	1543.546	-53.750
1600	1149.223	2018.948	1262.368	1210.528	496.109	1613.428	-52.672
1700	1161.793	2089.005	1308.950	1326.094	497.771	1683.179	-51.717
1800	1172.719	2155.728	1354.154	1442.832	499.385	1752.912	-50.867
1900	1182.264	2219.395	1398.031	1560.592	500.924	1822.491	-50.103
2000	1190.643	2280.255	1440.632	1679.246	502.335	1892.025	-49.414
2100	1198.031	2338.529	1482.011	1798.687	503.524	1961.477	-48.788
2200	1204.573	2394.415	1522.223	1918.824	504.497	2030.876	-48.218
2300	1210.390	2448.092	1561.319	2039.578	505.255	2100.241	-47.697
2400	1215.582	2499.717	1599.350	2160.881	505.710	2169.512	-47.217
2500	1220.233	2549.436	1636.365	2282.676	505.885	2238.916	-46.779
2600	1224.413	2597.377	1672.411	2404.912	505.737	2308.169	-46.371
2700	1228.183	2643.658	1707.531	2527.545	505.274	2377.534	-45.995
2800	1231.593	2688.387	1741.767	2650.537	504.466	2446.940	-45.647
2900	1234.687	2731.660	1775.159	2773.853	503.278	2516.318	-45.323
3000	1237.501	2773.566	1807.745	2897.465	501.770	2585.779	-45.021
3100	1240.068	2814.186	1839.559	3021.345	499.842	2655.191	-44.739
3200	1242.416	2853.594	1870.635	3145.471	497.552	2724.770	-44.476
3300	1244.568	2891.859	1901.004	3269.822	494.879	2794.480	-44.232
3400	1246.545	2929.043	1930.696	3394.379	491.784	2864.158	-44.002
3500	1248.365	2965.204	1959.739	3519.126	488.278	2933.912	-43.785
3600	1250.045	3000.395	1988.160	3644.047	484.392	3003.891	-43.584
3700	1251.598	3034.666	2015.983	3769.130	480.083	3073.996	-43.396
3800	1253.036	3068.064	2043.231	3894.363	475.324	3144.156	-43.219
3900	1254.371	3100.629	2069.928	4019.734	470.163	3214.369	-43.051
4000	1255.611	3132.403	2096.095	4145.234	464.583	3284.906	-42.896
4100	1256.766	3163.422	2121.750	4270.853	458.538	3355.492	-42.749
4200	1257.843	3193.720	2146.914	4396.584	452.065	3426.220	-42.610
4300	1258.849	3223.329	2171.604	4522.420	445.148	3496.990	-42.479
4400	1259.789	3252.281	2195.837	4648.352	437.797	3568.042	-42.357
4500	1260.671	3280.602	2219.629	4774.376	430.032	3639.335	-42.243
4600	1261.497	3308.319	2242.996	4900.484	421.785	3710.826	-42.137
4700	1262.273	3335.457	2265.952	5026.673	413.078	3782.351	-42.035
4800	1263.003	3362.040	2288.512	5152.937	403.966	3854.205	-41.941
4900	1263.690	3388.090	2310.687	5279.272	394.357	3926.073	-41.852
5000	1264.337	3413.626	2332.491	5405.674	384.371	3998.380	-41.770

3.623. Tetrabenzo[bc,ef,hi,kl]coronene



Formula: $C_{36}H_{16}$
Mass: 448.512 g/mol
CAS Number: 128366-79-0
Point Group: C_{2v}

Length: 15.87 Å
Width: 12.89 Å
Breadth: 3.893 Å
L/B Ratio: 1.231

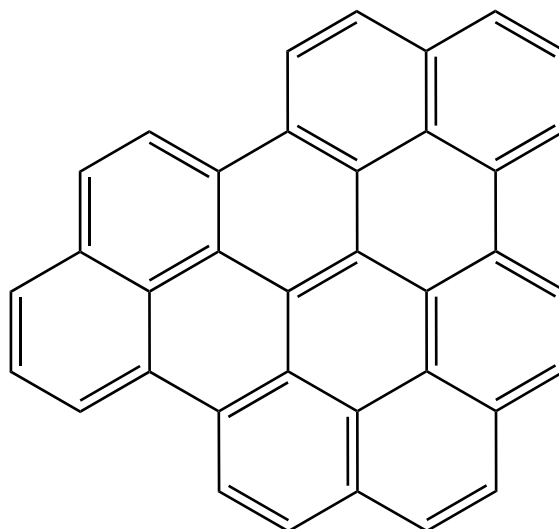
Cartesian coordinates:

C	2.8466	1.7185	0.0000	C	3.5272	-1.9970	0.0000	H	4.6355	2.9198	0.0000
C	3.5346	2.9305	0.0000	C	2.8383	-0.7653	0.0000	H	3.3989	5.0827	0.0000
C	2.8435	4.1391	0.0000	C	1.4082	-0.7559	0.0000	H	0.9090	5.1020	0.0000
C	1.4601	4.1491	0.0000	C	2.7913	-3.2195	0.0000	H	-0.8781	5.1074	0.0000
C	0.6989	0.4809	0.0000	C	-3.5671	0.4732	0.0000	H	-3.3680	5.1032	0.0000
C	1.4317	1.7220	0.0000	C	-4.9538	0.4382	0.0000	H	-4.6177	2.9479	0.0000
C	0.7355	2.9476	0.0000	C	-5.6414	-0.7824	0.0000	H	5.4703	-2.9619	0.0000
C	-0.7177	2.9520	0.0000	C	-4.9510	-1.9736	0.0000	H	6.7317	-0.8202	0.0000
C	-1.4349	4.1578	0.0000	C	-2.8429	-0.7482	0.0000	H	5.5228	1.3524	0.0000
C	-2.8183	4.1562	0.0000	C	-3.5392	-1.9757	0.0000	H	3.3455	-4.1663	0.0000
C	-3.5168	2.9519	0.0000	C	-2.8107	-3.2026	0.0000	H	-5.5146	1.3856	0.0000
C	-1.4213	1.7306	0.0000	C	-1.4128	-0.7474	0.0000	H	-6.7365	-0.7797	0.0000
C	-2.8361	1.7357	0.0000	C	-0.7164	-1.9643	0.0000	H	-5.4881	-2.9289	0.0000
C	-0.6960	0.4851	0.0000	C	-1.4407	-3.2051	0.0000	H	-3.3706	-4.1461	0.0000
C	3.5698	0.4516	0.0000	C	-0.6862	-4.4443	0.0000	H	-1.2540	-5.3821	0.0000
C	4.9389	-2.0035	0.0000	C	0.6594	-4.4483	0.0000	H	1.2215	-5.3895	0.0000
C	5.6366	-0.8164	0.0000	C	1.4213	-3.2137	0.0000				
C	4.9563	0.4083	0.0000	C	0.7046	-1.9686	0.0000				

Table 3.623: Table of thermodynamic data as a function of temperature for Tetra-benzo[bc,ef,hi,kl]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-59.578	524.358	524.358	∞
100	122.227	361.319	885.411	-52.409	551.369	599.246	-313.008
200	262.832	487.141	654.405	-33.453	537.037	652.859	-170.506
250	342.251	554.276	627.620	-18.336	530.330	682.587	-142.616
298.15	419.130	621.151	621.151	0.000	524.358	712.470	-124.819
300	422.045	623.753	621.159	0.778	524.136	713.634	-124.252
350	498.666	694.624	626.581	23.815	518.625	745.666	-111.282
400	569.788	765.924	639.543	50.552	513.835	778.424	-101.650
450	634.297	836.827	657.531	80.683	509.669	811.753	-94.224
500	691.995	906.702	678.965	113.868	506.031	845.544	-88.332
600	788.631	1041.764	728.274	188.094	500.017	914.041	-79.573
700	864.657	1169.271	782.260	270.908	495.498	983.430	-73.383
800	925.133	1288.827	838.191	360.509	492.319	1053.354	-68.776
900	973.953	1400.709	894.546	455.547	490.305	1123.595	-65.210
1000	1013.905	1505.461	950.457	555.005	489.303	1194.022	-62.368
1100	1046.979	1603.696	1005.424	658.099	489.102	1264.522	-60.046
1200	1074.626	1696.016	1059.166	764.220	489.562	1334.987	-58.109
1300	1097.927	1782.978	1111.532	872.880	490.490	1405.407	-56.469
1400	1117.709	1865.086	1162.452	983.688	491.746	1475.747	-55.060
1500	1134.614	1942.792	1211.908	1096.326	493.256	1545.993	-53.835
1600	1149.150	2016.494	1259.911	1210.532	494.874	1616.120	-52.760
1700	1161.719	2086.547	1306.493	1326.091	496.529	1686.117	-51.807
1800	1172.646	2153.265	1351.698	1442.821	498.136	1756.096	-50.960
1900	1182.192	2216.928	1395.574	1560.574	499.668	1825.921	-50.197
2000	1190.573	2277.784	1438.174	1679.221	501.071	1895.702	-49.510
2100	1197.964	2336.055	1479.553	1798.655	502.254	1965.401	-48.886
2200	1204.509	2391.939	1519.763	1918.785	503.220	2035.048	-48.317
2300	1210.328	2445.612	1558.859	2039.533	503.971	2104.661	-47.797
2400	1215.523	2497.235	1596.889	2160.830	504.421	2174.180	-47.319
2500	1220.176	2546.951	1633.903	2282.619	504.590	2243.832	-46.881
2600	1224.359	2594.890	1669.948	2404.850	504.436	2313.334	-46.474
2700	1228.131	2641.170	1705.067	2527.478	503.968	2382.947	-46.100
2800	1231.544	2685.897	1739.302	2650.464	503.154	2452.602	-45.753
2900	1234.639	2729.168	1772.694	2773.776	501.962	2522.230	-45.429
3000	1237.456	2771.072	1805.278	2897.383	500.449	2591.940	-45.129
3100	1240.025	2811.691	1837.091	3021.259	498.517	2661.601	-44.847
3200	1242.375	2851.098	1868.166	3145.380	496.223	2731.430	-44.585
3300	1244.529	2889.361	1898.535	3269.727	493.545	2801.390	-44.341
3400	1246.508	2926.544	1928.226	3394.280	490.447	2871.318	-44.112
3500	1248.330	2962.704	1957.268	3519.023	486.938	2941.321	-43.896
3600	1250.011	2997.894	1985.688	3643.942	483.048	3011.551	-43.696
3700	1251.565	3032.165	2013.510	3769.021	478.736	3081.906	-43.508
3800	1253.005	3065.561	2040.758	3894.251	473.973	3152.316	-43.331
3900	1254.341	3098.126	2067.454	4019.619	468.809	3222.779	-43.163
4000	1255.582	3129.899	2093.620	4145.116	463.226	3293.567	-43.009
4100	1256.738	3160.917	2119.275	4270.732	457.179	3364.403	-42.862
4200	1257.816	3191.214	2144.438	4396.461	450.703	3435.382	-42.724
4300	1258.823	3220.823	2169.127	4522.293	443.784	3506.402	-42.593
4400	1259.765	3249.774	2193.359	4648.223	436.430	3577.705	-42.472
4500	1260.647	3278.094	2217.151	4774.244	428.663	3649.248	-42.358
4600	1261.474	3305.811	2240.517	4900.351	420.413	3720.991	-42.252
4700	1262.251	3332.949	2263.473	5026.538	411.704	3792.766	-42.151
4800	1262.982	3359.532	2286.032	5152.800	402.590	3864.871	-42.057
4900	1263.669	3385.580	2308.206	5279.133	392.979	3936.990	-41.968
5000	1264.317	3411.117	2330.010	5405.532	382.990	4009.548	-41.887

3.624. Dinaphtho[8,1,2-*abc*:2',1',8'-*efg*]coronene



Formula: $C_{36}H_{16}$
Mass: 448.512 g/mol
CAS Number: 122677-68-3
Point Group: C_{2v}

Length: 15.88 Å
Width: 12.88 Å
Breadth: 3.893 Å
L/B Ratio: 1.233

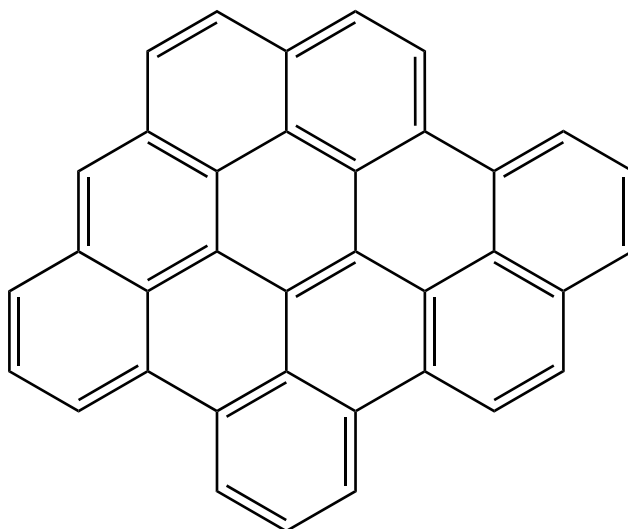
Cartesian coordinates:

C	-0.7001	-0.0591	0.0000	C	-5.6660	-1.2194	0.0000	H	4.6531	2.3285	0.0000
C	0.6977	-0.0831	0.0000	C	-4.9960	-2.4282	0.0000	H	3.4442	4.5044	0.0000
C	1.4504	1.1472	0.0000	C	-2.8658	-1.2455	0.0000	H	1.3408	5.7697	0.0000
C	2.8512	1.1353	0.0000	C	-3.5913	-2.4555	0.0000	H	-1.1422	5.8122	0.0000
C	3.5523	2.3584	0.0000	C	-2.8767	-3.7003	0.0000	H	-3.2877	4.6198	0.0000
C	2.8851	3.5617	0.0000	C	-1.5221	-3.7226	0.0000	H	-4.5705	2.4866	0.0000
C	0.7576	2.3856	0.0000	C	-0.7543	-2.5095	0.0000	H	-5.4941	0.9425	0.0000
C	1.4764	3.5954	0.0000	C	-1.4305	-1.2777	0.0000	H	-6.7609	-1.1984	0.0000
C	0.7613	4.8394	0.0000	C	3.5616	-0.1340	0.0000	H	-5.5535	-3.3717	0.0000
C	-0.5949	4.8626	0.0000	C	4.9098	-2.5981	0.0000	H	-3.4554	-4.6312	0.0000
C	-0.6754	2.4101	0.0000	C	5.6209	-1.4129	0.0000	H	-0.9700	-4.6750	0.0000
C	-1.3523	3.6439	0.0000	C	4.9528	-0.1880	0.0000	H	5.4347	-3.5600	0.0000
C	-2.7612	3.6585	0.0000	C	3.5050	-2.5772	0.0000	H	6.7158	-1.4295	0.0000
C	-3.4693	2.4788	0.0000	C	2.8214	-1.3430	0.0000	H	5.5231	0.7537	0.0000
C	-2.8106	1.2324	0.0000	C	1.3859	-1.3260	0.0000	H	0.8092	-4.7055	0.0000
C	-1.4102	1.1962	0.0000	C	0.6678	-2.5339	0.0000	H	3.2946	-4.7469	0.0000
C	-3.5641	-0.0118	0.0000	C	1.3936	-3.7726	0.0000				
C	-4.9563	-0.0181	0.0000	C	2.7481	-3.7967	0.0000				

Table 3.624: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*abc*:2',1',8'-*efg*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.396	497.714	497.714	∞
100	121.603	359.840	882.536	-52.270	524.865	572.889	-299.240
200	262.078	485.095	652.074	-33.396	510.450	626.681	-163.669
250	341.684	552.083	625.329	-18.312	503.710	656.516	-137.169
298.15	418.679	618.869	618.869	0.000	497.714	686.506	-120.271
300	421.596	621.468	618.877	0.777	497.491	687.675	-119.732
350	498.284	692.275	624.294	23.793	491.960	719.822	-107.425
400	569.446	763.527	637.245	50.513	487.151	752.699	-98.290
450	633.986	834.392	655.220	80.627	482.969	786.149	-91.252
500	691.710	904.235	676.640	113.798	479.316	820.062	-85.670
600	788.391	1039.250	725.921	187.997	473.275	888.808	-77.376
700	864.457	1166.723	779.881	270.789	468.735	958.450	-71.519
800	924.966	1286.254	835.789	360.372	465.538	1028.631	-67.161
900	973.813	1398.118	892.124	455.395	463.509	1099.130	-63.791
1000	1013.787	1502.857	948.017	554.839	462.493	1169.817	-61.104
1100	1046.879	1601.081	1002.969	657.923	462.281	1240.578	-58.909
1200	1074.540	1693.393	1056.697	764.034	462.733	1311.305	-57.078
1300	1097.852	1780.348	1109.051	872.687	463.653	1381.988	-55.528
1400	1117.644	1862.452	1159.960	983.488	464.902	1452.591	-54.196
1500	1134.557	1940.153	1209.407	1096.120	466.406	1523.100	-53.038
1600	1149.100	2013.851	1257.401	1210.320	468.018	1593.491	-52.021
1700	1161.674	2083.901	1303.976	1325.874	469.668	1663.752	-51.120
1800	1172.605	2150.617	1349.173	1442.600	471.270	1733.997	-50.318
1900	1182.156	2214.279	1393.042	1560.349	472.799	1804.086	-49.597
2000	1190.540	2275.133	1435.637	1678.993	474.199	1874.133	-48.946
2100	1197.934	2333.402	1477.010	1798.424	475.378	1944.097	-48.356
2200	1204.481	2389.284	1517.216	1918.551	476.341	2014.009	-47.818
2300	1210.303	2442.957	1556.306	2039.296	477.090	2083.887	-47.326
2400	1215.500	2494.579	1594.332	2160.591	477.537	2153.672	-46.872
2500	1220.155	2544.294	1631.342	2282.378	477.704	2223.590	-46.458
2600	1224.339	2592.232	1667.383	2404.607	477.549	2293.357	-46.073
2700	1228.113	2638.511	1702.499	2527.232	477.079	2363.236	-45.719
2800	1231.527	2683.237	1736.731	2650.217	476.263	2433.157	-45.390
2900	1234.624	2726.508	1770.119	2773.527	475.069	2503.051	-45.084
3000	1237.441	2768.412	1802.701	2897.133	473.555	2573.027	-44.799
3100	1240.012	2809.030	1834.512	3021.007	471.621	2642.954	-44.533
3200	1242.362	2848.436	1865.584	3145.128	469.326	2713.049	-44.285
3300	1244.517	2886.699	1895.950	3269.473	466.647	2783.276	-44.055
3400	1246.496	2923.882	1925.639	3394.025	463.547	2853.469	-43.837
3500	1248.319	2960.041	1954.679	3518.767	460.037	2923.739	-43.634
3600	1250.001	2995.231	1983.097	3643.684	456.146	2994.235	-43.444
3700	1251.556	3029.502	2010.917	3768.763	451.833	3064.856	-43.267
3800	1252.996	3062.898	2038.163	3893.992	447.070	3135.533	-43.100
3900	1254.332	3095.462	2064.858	4019.359	441.905	3206.262	-42.942
4000	1255.574	3127.235	2091.021	4144.855	436.321	3277.316	-42.796
4100	1256.731	3158.253	2116.675	4270.471	430.273	3348.419	-42.659
4200	1257.809	3188.550	2141.836	4396.198	423.796	3419.664	-42.529
4300	1258.816	3218.159	2166.524	4522.030	416.876	3490.951	-42.406
4400	1259.758	3247.109	2190.755	4647.959	409.521	3562.520	-42.292
4500	1260.641	3275.430	2214.545	4773.980	401.754	3634.330	-42.185
4600	1261.468	3303.146	2237.910	4900.086	393.504	3706.339	-42.086
4700	1262.245	3330.284	2260.865	5026.272	384.794	3778.380	-41.991
4800	1262.976	3356.867	2283.422	5152.533	375.679	3850.752	-41.904
4900	1263.664	3382.915	2305.596	5278.866	366.068	3923.137	-41.820
5000	1264.312	3408.451	2327.398	5405.265	356.079	3995.962	-41.745

3.625. Dibenzo[*ef,hi*]naphtho[8,1,2-*abc*]coronene



Formula: $C_{36}H_{16}$
Mass: 448.512 g/mol
CAS Number: 128395-03-9
Point Group: C_s

Length: 15.89 Å
Width: 12.89 Å
Breadth: 3.891 Å
L/B Ratio: 1.233

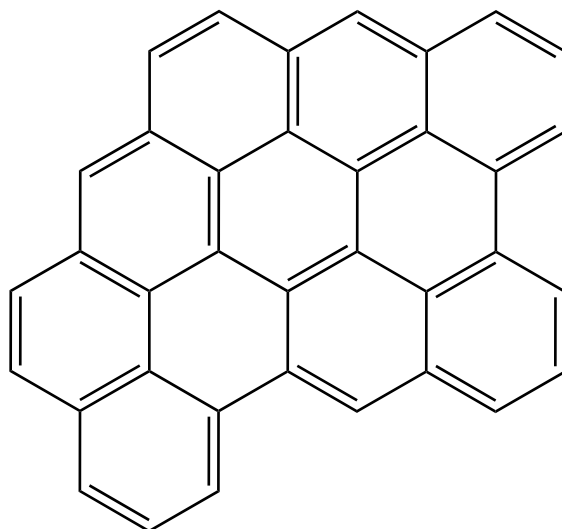
Cartesian coordinates:

C	2.2067	-4.1507	0.0000	C	1.3271	4.6618	0.0000	H	3.0534	-4.8469	0.0000
C	0.9352	-4.6022	0.0000	C	0.0296	4.2037	0.0000	H	0.7168	-5.6764	0.0000
C	2.5003	-2.7346	0.0000	C	0.8271	1.9044	0.0000	H	4.6386	-2.9756	0.0000
C	3.7981	-2.2705	0.0000	C	-0.2460	2.8193	0.0000	H	6.2289	-1.1199	0.0000
C	4.0692	-0.8793	0.0000	C	0.5622	0.4956	0.0000	H	6.6812	1.3248	0.0000
C	5.4041	-0.3983	0.0000	C	-0.7476	0.0263	0.0000	H	4.8034	2.9530	0.0000
C	5.6522	0.9501	0.0000	C	-2.3387	-1.8758	0.0000	H	-3.5961	-3.6250	0.0000
C	4.5896	1.8729	0.0000	C	-1.0158	-1.3853	0.0000	H	-1.6959	-5.2306	0.0000
C	-0.1827	-3.6883	0.0000	C	-3.4536	-0.9367	0.0000	H	3.4316	4.1259	0.0000
C	-2.5585	-3.2559	0.0000	C	-5.5889	0.8897	0.0000	H	1.5335	5.7371	0.0000
C	-1.4993	-4.1524	0.0000	C	-5.8324	-0.4654	0.0000	H	-0.8153	4.9091	0.0000
C	0.0645	-2.2968	0.0000	C	-4.7688	-1.3771	0.0000	H	-6.4185	1.6056	0.0000
C	1.4111	-1.8089	0.0000	C	-4.2624	1.3707	0.0000	H	-6.8608	-0.8417	0.0000
C	1.6603	-0.4328	0.0000	C	-3.1869	0.4592	0.0000	H	-4.9715	-2.4593	0.0000
C	3.0002	0.0447	0.0000	C	-1.8419	0.9533	0.0000	H	-2.4929	4.3097	0.0000
C	3.2766	1.4431	0.0000	C	-1.6006	2.3278	0.0000	H	-4.8344	3.4716	0.0000
C	2.1637	2.3887	0.0000	C	-2.7088	3.2302	0.0000				
C	2.3946	3.7560	0.0000	C	-3.9891	2.7740	0.0000				

Table 3.625: Table of thermodynamic data as a function of temperature for Dibenzo[*ef,hi*]naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.839	523.252	523.252	∞
100	123.271	371.094	896.434	-52.534	550.138	597.038	-311.854
200	263.436	497.458	664.967	-33.502	535.882	649.640	-169.665
250	342.751	564.716	638.146	-18.357	529.203	678.850	-141.835
298.15	419.525	631.671	631.671	0.000	523.252	708.227	-124.076
300	422.435	634.275	631.679	0.779	523.031	709.372	-123.510
350	498.962	705.199	637.105	23.833	517.537	740.877	-110.567
400	570.011	776.533	650.076	50.583	512.759	773.104	-100.955
450	634.468	847.459	668.074	80.723	508.604	805.903	-93.545
500	692.130	917.350	689.518	113.916	504.972	839.161	-87.665
600	788.722	1052.433	738.844	188.153	498.970	906.592	-78.924
700	864.725	1179.952	792.845	270.975	494.459	974.914	-72.747
800	925.186	1299.516	848.788	360.582	491.286	1043.769	-68.150
900	973.997	1411.404	905.154	455.625	489.277	1112.941	-64.592
1000	1013.942	1516.160	961.074	555.086	488.279	1182.298	-61.756
1100	1047.011	1614.398	1016.049	658.185	488.081	1251.729	-59.438
1200	1074.653	1706.720	1069.797	764.308	488.544	1321.123	-57.506
1300	1097.950	1793.684	1122.168	872.971	489.475	1390.473	-55.869
1400	1117.729	1875.794	1173.094	983.781	490.733	1459.742	-54.463
1500	1134.632	1953.501	1222.554	1096.421	492.245	1528.917	-53.241
1600	1149.166	2027.204	1270.561	1210.628	493.865	1597.973	-52.167
1700	1161.733	2097.258	1317.147	1326.188	495.521	1666.899	-51.217
1800	1172.658	2163.977	1362.355	1442.920	497.129	1735.807	-50.371
1900	1182.204	2227.641	1406.234	1560.674	498.662	1804.561	-49.610
2000	1190.584	2288.498	1448.837	1679.322	500.067	1873.271	-48.924
2100	1197.973	2346.769	1490.218	1798.758	501.250	1941.898	-48.301
2200	1204.517	2402.653	1530.431	1918.889	502.217	2010.473	-47.734
2300	1210.336	2456.327	1569.528	2039.637	502.969	2079.015	-47.215
2400	1215.530	2507.950	1607.560	2160.935	503.420	2147.463	-46.737
2500	1220.183	2557.666	1644.576	2282.725	503.589	2216.043	-46.301
2600	1224.365	2605.606	1680.623	2404.956	503.437	2284.474	-45.895
2700	1228.137	2651.886	1715.743	2527.585	502.969	2353.015	-45.521
2800	1231.549	2696.613	1749.980	2650.572	502.156	2421.599	-45.175
2900	1234.645	2739.884	1783.373	2773.884	500.964	2490.154	-44.852
3000	1237.461	2781.789	1815.958	2897.491	499.452	2558.793	-44.552
3100	1240.030	2822.408	1847.773	3021.368	497.520	2627.383	-44.270
3200	1242.379	2861.815	1878.849	3145.490	495.226	2696.140	-44.009
3300	1244.533	2900.078	1909.218	3269.837	492.549	2765.028	-43.766
3400	1246.511	2937.261	1938.911	3394.391	489.451	2833.884	-43.536
3500	1248.333	2973.421	1967.954	3519.134	485.942	2902.816	-43.321
3600	1250.014	3008.611	1996.374	3644.053	482.053	2971.974	-43.121
3700	1251.568	3042.882	2024.197	3769.133	477.741	3041.257	-42.934
3800	1253.008	3076.278	2051.446	3894.363	472.979	3110.595	-42.757
3900	1254.343	3108.843	2078.143	4019.731	467.815	3179.987	-42.590
4000	1255.585	3140.616	2104.309	4145.228	462.232	3249.703	-42.436
4100	1256.741	3171.634	2129.965	4270.845	456.185	3319.468	-42.290
4200	1257.819	3201.932	2155.129	4396.574	449.710	3389.374	-42.152
4300	1258.826	3231.541	2179.819	4522.406	442.791	3459.323	-42.022
4400	1259.767	3260.492	2204.051	4648.337	435.437	3529.554	-41.900
4500	1260.649	3288.812	2227.844	4774.358	427.670	3600.025	-41.787
4600	1261.476	3316.529	2251.211	4900.465	419.421	3670.696	-41.681
4700	1262.253	3343.667	2274.167	5026.652	410.712	3741.400	-41.580
4800	1262.984	3370.249	2296.726	5152.914	401.598	3812.432	-41.487
4900	1263.671	3396.298	2318.901	5279.247	391.987	3883.480	-41.398
5000	1264.319	3421.835	2340.705	5405.647	381.999	3954.966	-41.316

3.626. Dibenzo[*kl,no*]naphtho[8,1,2-*abc*]coronene



Formula: $C_{36}H_{16}$
Mass: 448.512 g/mol
CAS Number: 128345-75-5
Point Group: C_s

Length: 15.92 Å
Width: 12.88 Å
Breadth: 3.893 Å
L/B Ratio: 1.235

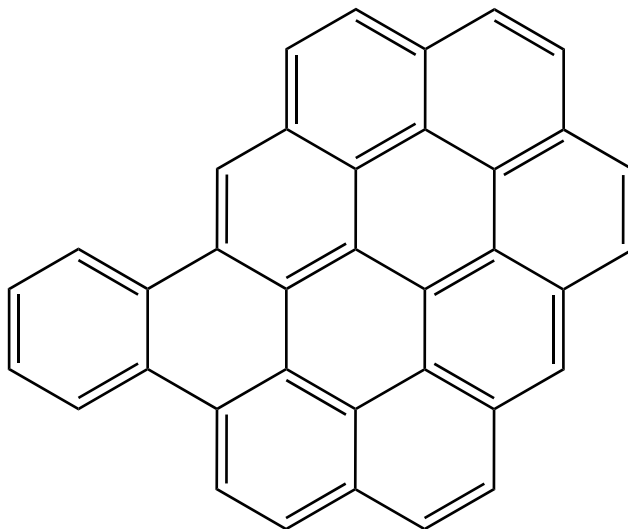
Cartesian coordinates:

C	4.7074	-2.0504	0.0000	C	-3.7297	0.7087	0.0000	H	5.1941	-3.0325	0.0000
C	5.4394	-0.9099	0.0000	C	-5.1120	0.7231	0.0000	H	6.5350	-0.9440	0.0000
C	2.7568	1.7187	0.0000	C	-5.8451	-0.4769	0.0000	H	6.6567	1.5002	0.0000
C	3.3960	0.4536	0.0000	C	-5.2003	-1.6884	0.0000	H	5.5220	3.7119	0.0000
C	4.8027	0.3780	0.0000	C	-3.0446	-0.5407	0.0000	H	3.0372	3.8513	0.0000
C	5.5626	1.5624	0.0000	C	-3.7839	-1.7439	0.0000	H	1.2277	3.9328	0.0000
C	4.9314	2.7898	0.0000	C	-3.1033	-2.9906	0.0000	H	-0.8517	5.2399	0.0000
C	3.5355	2.8695	0.0000	C	-1.6209	-0.5936	0.0000	H	-3.3364	5.3317	0.0000
C	0.5403	0.5744	0.0000	C	3.2716	-2.0051	0.0000	H	-4.6739	3.2325	0.0000
C	1.2979	1.7905	0.0000	C	2.6249	-0.7574	0.0000	H	-5.6386	1.6901	0.0000
C	0.6425	2.9987	0.0000	C	1.2083	-0.6946	0.0000	H	-6.9393	-0.4318	0.0000
C	-0.7771	3.0697	0.0000	C	2.5108	-3.1917	0.0000	H	-5.7694	-2.6250	0.0000
C	-1.4445	4.3183	0.0000	C	1.1277	-3.1418	0.0000	H	-3.6929	-3.9158	0.0000
C	-2.8172	4.3675	0.0000	C	0.4617	-1.8842	0.0000	H	3.0270	-4.1597	0.0000
C	-3.5739	3.1837	0.0000	C	-0.9683	-1.8294	0.0000	H	-1.6135	-5.2225	0.0000
C	-1.5329	1.8788	0.0000	C	-1.7282	-3.0416	0.0000	H	0.8616	-5.3092	0.0000
C	-2.9550	1.9462	0.0000	C	-1.0166	-4.3030	0.0000				
C	-0.8561	0.6226	0.0000	C	0.3304	-4.3502	0.0000				

Table 3.626: Table of thermodynamic data as a function of temperature for Dibenzo[*kl,no*]naphtho[8,1,2-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.468	519.400	519.400	∞
100	121.543	365.370	889.095	-52.372	546.447	593.919	-310.225
200	262.664	490.836	658.159	-33.464	532.067	647.150	-169.015
250	342.394	557.970	631.361	-18.348	525.360	676.694	-141.384
298.15	419.459	624.887	624.887	0.000	519.400	706.397	-123.755
300	422.378	627.491	624.896	0.779	519.178	707.555	-123.194
350	499.087	698.421	630.322	23.835	513.686	739.398	-110.347
400	570.233	769.779	643.295	50.594	508.918	771.964	-100.806
450	634.735	840.735	661.297	80.747	504.775	805.100	-93.452
500	692.414	910.655	682.748	113.953	501.157	838.694	-87.616
600	789.011	1045.790	732.091	188.219	495.183	906.792	-78.942
700	865.013	1173.354	786.111	271.070	490.701	975.775	-72.812
800	925.478	1292.956	842.074	360.705	487.557	1045.288	-68.249
900	974.291	1404.879	898.459	455.778	485.578	1115.114	-64.718
1000	1014.236	1509.666	954.397	555.269	484.609	1185.123	-61.903
1100	1047.302	1607.932	1009.390	658.396	484.440	1255.201	-59.603
1200	1074.937	1700.279	1063.155	764.549	484.932	1325.241	-57.685
1300	1098.225	1787.265	1115.543	873.239	485.891	1395.234	-56.060
1400	1117.993	1869.396	1166.484	984.077	487.176	1465.144	-54.664
1500	1134.884	1947.120	1215.959	1096.742	488.714	1534.957	-53.451
1600	1149.404	2020.839	1263.980	1210.974	490.358	1604.651	-52.385
1700	1161.959	2090.907	1310.579	1326.557	492.037	1674.212	-51.441
1800	1172.871	2157.639	1355.799	1443.311	493.667	1743.755	-50.601
1900	1182.404	2221.314	1399.690	1561.086	495.222	1813.142	-49.846
2000	1190.772	2282.180	1442.304	1679.754	496.645	1882.484	-49.164
2100	1198.150	2340.461	1483.695	1799.207	497.847	1951.743	-48.546
2200	1204.684	2396.352	1523.918	1919.355	498.831	2020.949	-47.982
2300	1210.493	2450.033	1563.025	2040.120	499.600	2090.120	-47.467
2400	1215.678	2501.663	1601.066	2161.433	500.065	2159.197	-46.993
2500	1220.322	2551.385	1638.090	2283.238	500.249	2228.406	-46.559
2600	1224.497	2599.330	1674.145	2405.482	500.110	2297.464	-46.156
2700	1228.261	2645.615	1709.273	2528.123	499.655	2366.633	-45.784
2800	1231.666	2690.346	1743.517	2651.122	498.854	2435.843	-45.440
2900	1234.755	2733.622	1776.916	2774.446	497.674	2505.025	-45.119
3000	1237.566	2775.530	1809.509	2898.064	496.172	2574.290	-44.821
3100	1240.129	2816.152	1841.329	3021.951	494.251	2643.505	-44.542
3200	1242.474	2855.562	1872.411	3146.083	491.967	2712.887	-44.282
3300	1244.622	2893.829	1902.786	3270.439	489.299	2782.401	-44.041
3400	1246.597	2931.014	1932.484	3395.001	486.209	2851.882	-43.813
3500	1248.414	2967.176	1961.533	3519.753	482.709	2921.438	-43.599
3600	1250.092	3002.369	1989.958	3644.680	478.827	2991.220	-43.401
3700	1251.642	3036.642	2017.786	3769.767	474.523	3061.128	-43.214
3800	1253.078	3070.040	2045.039	3895.004	469.768	3131.090	-43.039
3900	1254.411	3102.607	2071.740	4020.380	464.611	3201.105	-42.873
4000	1255.649	3134.382	2097.911	4145.883	459.035	3271.445	-42.720
4100	1256.802	3165.401	2123.570	4271.507	452.994	3341.833	-42.575
4200	1257.878	3195.700	2148.738	4397.241	446.525	3412.363	-42.438
4300	1258.882	3225.310	2173.431	4523.080	439.611	3482.934	-42.308
4400	1259.821	3254.262	2197.668	4649.015	432.263	3553.788	-42.188
4500	1260.701	3282.584	2221.464	4775.042	424.502	3624.883	-42.076
4600	1261.526	3310.302	2244.834	4901.154	416.258	3696.176	-41.971
4700	1262.301	3337.441	2267.793	5027.346	407.553	3767.502	-41.870
4800	1263.030	3364.025	2290.355	5153.612	398.444	3839.158	-41.778
4900	1263.716	3390.075	2312.534	5279.950	388.838	3910.828	-41.689
5000	1264.362	3415.612	2334.341	5406.354	378.854	3982.936	-41.609

3.627. Benz[*a*]ovalene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 75449-88-6
Point Group: C_s

Length: 15.91 Å
Width: 12.88 Å
Breadth: 3.886 Å
L/B Ratio: 1.235

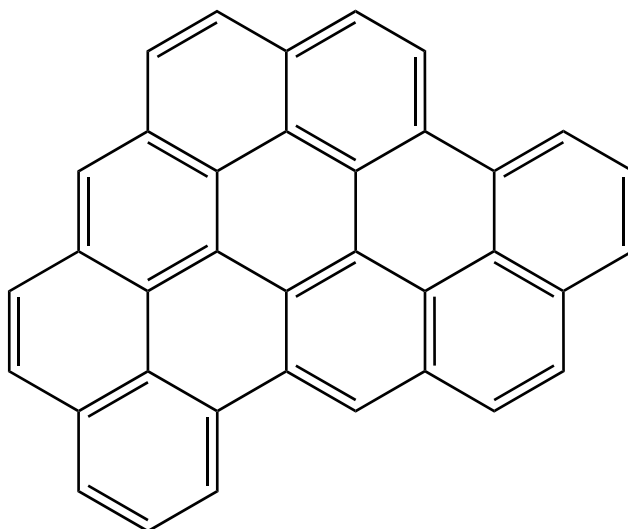
Cartesian coordinates:

C	1.0783	-2.8227	0.0000	C	-2.4215	0.8832	0.0000	H	1.6234	-3.7804	0.0000
C	-0.2959	-0.3793	0.0000	C	-3.1192	2.1126	0.0000	H	-2.9469	4.2693	0.0000
C	1.1086	-0.3944	0.0000	C	-4.5564	2.0910	0.0000	H	5.0245	2.0723	0.0000
C	1.7991	-1.6328	0.0000	C	-5.2413	0.9196	0.0000	H	3.7883	4.2284	0.0000
C	-1.0111	0.8708	0.0000	C	-4.5533	-0.3401	0.0000	H	1.6677	5.4693	0.0000
C	-2.4034	3.3164	0.0000	C	-3.1513	-0.3499	0.0000	H	-0.8123	5.4870	0.0000
C	1.8379	0.8470	0.0000	C	-0.3247	-2.8233	0.0000	H	-6.3503	-1.5540	0.0000
C	3.2413	0.8518	0.0000	C	-1.0174	-1.5952	0.0000	H	-5.1267	-3.7125	0.0000
C	3.9235	2.0826	0.0000	C	-2.4497	-1.5862	0.0000	H	-5.0861	3.0507	0.0000
C	3.2393	3.2798	0.0000	C	-3.1620	-2.7947	0.0000	H	-6.3373	0.9097	0.0000
C	-1.0088	3.3145	0.0000	C	-2.4358	-4.0316	0.0000	H	-3.0069	-4.9671	0.0000
C	-0.3032	2.0849	0.0000	C	-1.0781	-4.0455	0.0000	H	-0.5264	-4.9926	0.0000
C	1.1310	2.0770	0.0000	C	3.9611	-0.4120	0.0000	H	3.4132	-3.7846	0.0000
C	1.8337	3.2960	0.0000	C	3.2553	-1.6285	0.0000	H	5.9024	-3.7898	0.0000
C	1.0979	4.5329	0.0000	C	3.9741	-2.8372	0.0000	H	7.1514	-1.6372	0.0000
C	-0.2557	4.5427	0.0000	C	5.3550	-2.8417	0.0000	H	5.9114	0.5212	0.0000
C	-5.2543	-1.5696	0.0000	C	6.0566	-1.6324	0.0000				
C	-4.5771	-2.7641	0.0000	C	5.3674	-0.4359	0.0000				

Table 3.627: Table of thermodynamic data as a function of temperature for Benz[*a*]ovalene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-59.239	484.917	484.917	∞
100	120.680	363.317	885.354	-52.204	512.134	559.811	-292.409
200	261.789	488.096	655.069	-33.395	497.655	613.285	-160.170
250	341.694	555.053	628.322	-18.317	490.908	642.971	-134.339
298.15	418.881	621.859	621.859	0.000	484.917	672.818	-117.872
300	421.805	624.459	621.867	0.778	484.695	673.981	-117.348
350	498.606	695.308	627.287	23.807	479.177	705.978	-105.359
400	569.824	766.607	640.246	50.545	474.386	738.702	-96.463
450	634.385	837.517	658.232	80.678	470.224	771.997	-89.609
500	692.114	907.403	679.666	113.869	466.590	805.753	-84.175
600	788.787	1042.491	728.976	188.109	460.590	874.178	-76.102
700	864.844	1170.024	782.968	270.939	456.089	943.493	-70.403
800	925.347	1289.607	838.906	360.561	452.930	1013.341	-66.163
900	974.188	1401.516	895.270	455.621	450.939	1083.502	-62.884
1000	1014.154	1506.293	951.190	555.103	449.961	1153.847	-60.270
1100	1047.235	1604.552	1006.168	658.223	449.785	1224.264	-58.134
1200	1074.882	1696.894	1059.920	764.370	450.271	1294.641	-56.353
1300	1098.179	1783.877	1112.296	873.055	451.224	1364.973	-54.844
1400	1117.954	1866.004	1163.226	983.888	452.506	1435.222	-53.548
1500	1134.850	1943.726	1212.692	1096.550	454.039	1505.375	-52.421
1600	1149.375	2017.442	1260.705	1210.779	455.681	1575.408	-51.431
1700	1161.933	2087.509	1307.297	1326.359	457.357	1645.309	-50.553
1800	1172.848	2154.239	1352.511	1443.111	458.984	1715.192	-49.773
1900	1182.384	2217.913	1396.395	1560.883	460.537	1784.918	-49.070
2000	1190.754	2278.779	1439.004	1679.549	461.958	1854.601	-48.436
2100	1198.134	2337.058	1480.391	1799.001	463.158	1924.200	-47.861
2200	1204.669	2392.949	1520.609	1919.148	464.141	1993.746	-47.337
2300	1210.480	2446.629	1559.712	2039.911	464.908	2063.258	-46.857
2400	1215.666	2498.259	1597.749	2161.223	465.372	2132.675	-46.415
2500	1220.311	2547.980	1634.770	2283.026	465.555	2202.224	-46.012
2600	1224.486	2595.925	1670.821	2405.269	465.415	2271.623	-45.637
2700	1228.252	2642.209	1705.946	2527.910	464.959	2341.132	-45.291
2800	1231.657	2686.940	1740.187	2650.908	464.157	2410.683	-44.971
2900	1234.747	2730.215	1773.584	2774.230	462.976	2480.206	-44.672
3000	1237.558	2772.123	1806.174	2897.848	461.473	2549.811	-44.395
3100	1240.122	2812.745	1837.992	3021.734	459.551	2619.367	-44.135
3200	1242.467	2852.155	1869.072	3145.865	457.266	2689.090	-43.894
3300	1244.616	2890.421	1899.445	3270.221	454.598	2758.945	-43.670
3400	1246.591	2927.606	1929.141	3394.782	451.508	2828.766	-43.458
3500	1248.409	2963.769	1958.188	3519.534	448.007	2898.663	-43.259
3600	1250.086	2998.961	1986.611	3644.460	444.125	2968.786	-43.075
3700	1251.637	3033.234	2014.437	3769.547	439.820	3039.034	-42.903
3800	1253.073	3066.632	2041.689	3894.783	435.065	3109.338	-42.740
3900	1254.406	3099.199	2068.389	4020.158	429.907	3179.694	-42.586
4000	1255.645	3130.973	2094.558	4145.661	424.331	3250.374	-42.445
4100	1256.798	3161.993	2120.216	4271.284	418.289	3321.103	-42.310
4200	1257.874	3192.292	2145.382	4397.018	411.820	3391.974	-42.184
4300	1258.878	3221.902	2170.075	4522.856	404.906	3462.886	-42.065
4400	1259.818	3250.854	2194.310	4648.792	397.557	3534.081	-41.954
4500	1260.698	3279.175	2218.105	4774.818	389.796	3605.516	-41.851
4600	1261.523	3306.893	2241.474	4900.930	381.551	3677.151	-41.754
4700	1262.298	3334.032	2264.432	5027.121	372.846	3748.818	-41.663
4800	1263.027	3360.616	2286.993	5153.388	363.737	3820.814	-41.578
4900	1263.713	3386.665	2309.171	5279.725	354.130	3892.825	-41.497
5000	1264.359	3412.202	2330.977	5406.129	344.146	3965.274	-41.424

3.628. Dinaphtho[8,1,2-*abc*:8',1',2'-*ghi*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 75459-02-8
Point Group: C_s

Length: 16.12 Å
Width: 12.75 Å
Breadth: 3.886 Å
L/B Ratio: 1.264

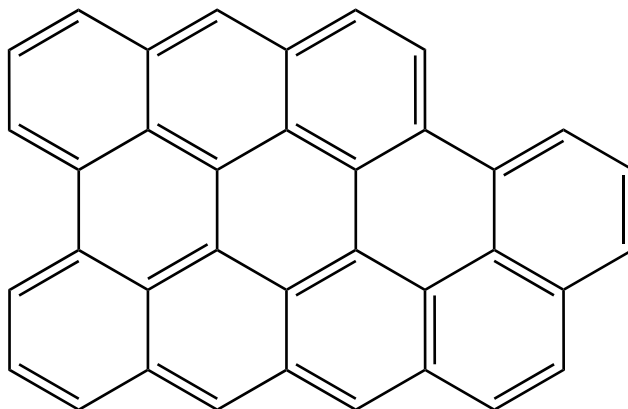
Cartesian coordinates:

C	0.0098	-2.8619	0.0000	C	-4.2218	-3.6036	0.0000	H	-0.3638	-3.8989	0.0000
C	-0.9091	-1.8148	0.0000	C	-2.8482	-3.3726	0.0000	H	4.3282	2.9390	0.0000
C	-0.4436	-0.4780	0.0000	C	-4.6375	-1.2249	0.0000	H	2.7056	4.8287	0.0000
C	0.9381	-0.2147	0.0000	C	-3.2473	-0.9848	0.0000	H	0.3882	5.6463	0.0000
C	1.4265	1.1412	0.0000	C	-2.7626	0.3675	0.0000	H	-2.0508	5.1913	0.0000
C	2.8037	1.4095	0.0000	C	-3.6757	1.4479	0.0000	H	-3.9136	3.5962	0.0000
C	3.2436	2.7477	0.0000	C	-5.0890	1.1658	0.0000	H	-6.1933	-2.7293	0.0000
C	2.3466	3.7931	0.0000	C	-5.5461	-0.1067	0.0000	H	-4.5960	-4.6327	0.0000
C	0.5006	2.2149	0.0000	C	3.7526	0.3079	0.0000	H	-2.1422	-4.2174	0.0000
C	0.9613	3.5436	0.0000	C	5.5562	-1.8465	0.0000	H	-5.7825	2.0147	0.0000
C	0.0066	4.6188	0.0000	C	6.0216	-0.5416	0.0000	H	-6.6214	-0.3196	0.0000
C	-1.3246	4.3702	0.0000	C	5.1298	0.5281	0.0000	H	6.2620	-2.6848	0.0000
C	-0.9090	1.9473	0.0000	C	4.1779	-2.1020	0.0000	H	7.0991	-0.3459	0.0000
C	-1.8291	3.0221	0.0000	C	3.2689	-1.0222	0.0000	H	5.5017	1.5644	0.0000
C	-3.2019	2.7613	0.0000	C	1.8583	-1.2851	0.0000	H	1.9542	-4.7209	0.0000
C	-1.3779	0.6186	0.0000	C	1.3871	-2.6148	0.0000	H	4.3947	-4.2716	0.0000
C	-2.3430	-2.0728	0.0000	C	2.3392	-3.6946	0.0000				
C	-5.1133	-2.5434	0.0000	C	3.6699	-3.4493	0.0000				

Table 3.628: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*abc*:8',1',2'-*ghi*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.695	493.978	493.978	∞
100	122.261	368.343	893.355	-52.501	520.896	568.071	-296.724
200	263.313	494.226	661.892	-33.533	506.576	620.981	-162.180
250	343.106	561.512	635.041	-18.382	499.903	650.351	-135.881
298.15	420.173	628.556	628.556	0.000	493.978	679.881	-119.110
300	423.091	631.164	628.564	0.780	493.758	681.032	-118.576
350	499.768	702.202	633.999	23.871	488.301	712.689	-106.361
400	570.869	773.648	646.990	50.663	483.565	745.064	-97.293
450	635.323	844.676	665.016	80.847	479.452	778.004	-90.306
500	692.954	914.655	686.492	114.081	475.863	811.400	-84.765
600	789.466	1049.881	735.886	188.397	469.939	879.092	-76.530
700	865.398	1177.509	789.954	271.289	465.499	947.663	-70.714
800	925.805	1297.159	845.959	360.961	462.390	1016.759	-66.386
900	974.572	1409.118	902.381	456.063	460.441	1086.163	-63.038
1000	1014.479	1513.933	958.352	555.580	459.498	1155.745	-60.369
1100	1047.514	1612.220	1013.374	658.731	459.352	1225.396	-58.188
1200	1075.123	1704.585	1067.166	764.903	459.864	1295.006	-56.369
1300	1098.390	1791.585	1119.577	873.611	460.840	1364.568	-54.828
1400	1118.139	1873.727	1170.539	984.464	462.141	1434.045	-53.504
1500	1135.015	1951.461	1220.032	1097.143	463.693	1503.425	-52.353
1600	1149.522	2025.188	1268.070	1211.388	465.349	1572.684	-51.342
1700	1162.065	2095.263	1314.685	1326.982	467.040	1641.810	-50.446
1800	1172.968	2162.000	1359.919	1443.746	468.680	1710.917	-49.649
1900	1182.492	2225.680	1403.822	1561.530	470.243	1779.868	-48.931
2000	1190.852	2286.551	1446.448	1680.206	471.676	1848.773	-48.284
2100	1198.224	2344.835	1487.851	1799.667	472.885	1917.594	-47.697
2200	1204.752	2400.730	1528.084	1919.823	473.876	1986.363	-47.161
2300	1210.556	2454.414	1567.199	2040.594	474.651	2055.096	-46.672
2400	1215.736	2506.046	1605.249	2161.913	475.123	2123.735	-46.221
2500	1220.376	2555.771	1642.282	2283.723	475.312	2192.505	-45.809
2600	1224.547	2603.718	1678.344	2405.973	475.178	2261.124	-45.426
2700	1228.308	2650.004	1713.479	2528.619	474.728	2329.855	-45.073
2800	1231.710	2694.737	1747.729	2651.622	473.932	2398.626	-44.746
2900	1234.796	2738.014	1781.135	2774.950	472.756	2467.369	-44.441
3000	1237.604	2779.924	1813.733	2898.572	471.258	2536.194	-44.158
3100	1240.165	2820.547	1845.559	3022.463	469.340	2604.970	-43.893
3200	1242.508	2859.958	1876.646	3146.598	467.060	2673.913	-43.646
3300	1244.654	2898.226	1907.026	3270.958	464.395	2742.987	-43.417
3400	1246.627	2935.412	1936.729	3395.523	461.309	2812.028	-43.201
3500	1248.443	2971.575	1965.782	3520.278	457.811	2881.144	-42.998
3600	1250.119	3006.769	1994.211	3645.207	453.933	2950.487	-42.810
3700	1251.668	3041.042	2022.043	3770.297	449.631	3019.954	-42.633
3800	1253.103	3074.441	2049.300	3895.537	444.878	3089.476	-42.467
3900	1254.434	3107.009	2076.005	4020.914	439.724	3159.051	-42.310
4000	1255.671	3138.784	2102.179	4146.420	434.150	3228.951	-42.165
4100	1256.823	3169.804	2127.842	4272.046	428.111	3298.899	-42.028
4200	1257.898	3200.103	2153.012	4397.782	421.644	3368.988	-41.899
4300	1258.901	3229.714	2177.709	4523.623	414.733	3439.119	-41.776
4400	1259.840	3258.667	2201.948	4649.561	407.386	3509.533	-41.663
4500	1260.719	3286.989	2225.747	4775.589	399.627	3580.187	-41.557
4600	1261.543	3314.707	2249.120	4901.702	391.384	3651.040	-41.458
4700	1262.317	3341.847	2272.081	5027.896	382.682	3721.926	-41.364
4800	1263.045	3368.430	2294.646	5154.164	373.574	3793.140	-41.277
4900	1263.730	3394.481	2316.827	5280.504	363.969	3864.370	-41.194
5000	1264.376	3420.018	2338.636	5406.909	353.987	3936.037	-41.119

3.629. Dibenzo[*hi,kl*]naphtho[8,1,2-*abc*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128345-77-7
Point Group: C_s

Length: 15.31 Å
Width: 11.69 Å
Breadth: 3.887 Å
L/B Ratio: 1.310

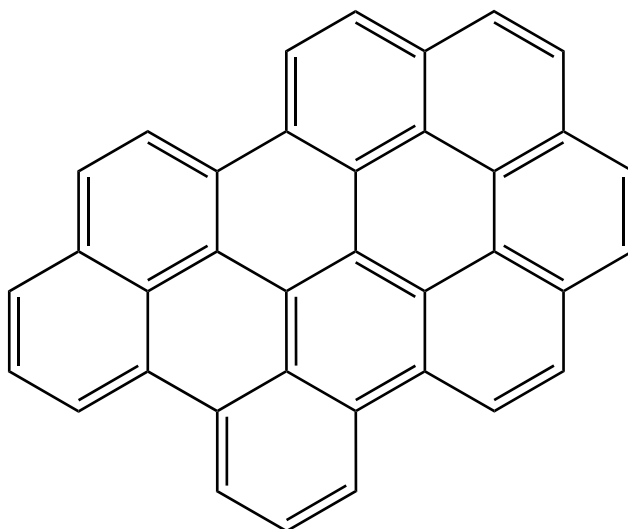
Cartesian coordinates:

C	5.0427	2.1329	0.0000	C	0.0296	1.2456	0.0000	H	6.0562	2.5506	0.0000
C	3.9612	2.9355	0.0000	C	-1.2602	0.6892	0.0000	H	4.0672	4.0266	0.0000
C	2.6174	2.3921	0.0000	C	-2.3939	1.5288	0.0000	H	1.6306	4.2979	0.0000
C	1.5165	3.2067	0.0000	C	-3.7178	0.9805	0.0000	H	-0.8055	4.5742	0.0000
C	0.1945	2.6599	0.0000	C	-3.8843	-0.4708	0.0000	H	-3.2342	4.8639	0.0000
C	-0.9290	3.4841	0.0000	C	-5.1336	-1.0498	0.0000	H	-5.5143	3.8733	0.0000
C	-2.2212	2.9368	0.0000	C	-5.2828	-2.4552	0.0000	H	-5.8178	1.4047	0.0000
C	-3.3752	3.7771	0.0000	C	-4.1869	-3.2709	0.0000	H	4.4976	-3.1873	0.0000
C	-4.6265	3.2321	0.0000	C	-2.7215	-1.3060	0.0000	H	6.7670	-2.1624	0.0000
C	-4.8014	1.8280	0.0000	C	-2.8745	-2.7143	0.0000	H	7.0337	0.3043	0.0000
C	4.9126	0.6904	0.0000	C	-1.7368	-3.5423	0.0000	H	-6.0264	-0.4054	0.0000
C	4.6216	-2.0935	0.0000	C	-1.4230	-0.7461	0.0000	H	-6.2928	-2.8785	0.0000
C	5.8765	-1.5249	0.0000	C	-0.2961	-1.5804	0.0000	H	-4.2969	-4.3612	0.0000
C	6.0285	-0.1324	0.0000	C	-0.4613	-2.9940	0.0000	H	-1.8649	-4.6319	0.0000
C	3.4634	-1.2874	0.0000	C	0.7123	-3.8254	0.0000	H	0.5757	-4.9129	0.0000
C	3.6119	0.1169	0.0000	C	1.9523	-3.2799	0.0000	H	2.8541	-3.9118	0.0000
C	2.4614	0.9621	0.0000	C	2.1437	-1.8572	0.0000				
C	1.1839	0.4015	0.0000	C	1.0272	-1.0228	0.0000				

Table 3.629: Table of thermodynamic data as a function of temperature for Dibenzo[hi,kl]naphtho[8,1,2-abc]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-59.941	550.538	550.538	∞
100	123.028	369.360	896.316	-52.696	577.262	624.335	-326.112
200	264.327	495.888	664.054	-33.633	563.037	677.109	-176.839
250	344.127	563.401	637.126	-18.431	556.414	706.390	-147.589
298.15	421.188	630.624	630.624	0.000	550.538	735.825	-128.911
300	424.106	633.239	630.632	0.782	550.320	736.972	-128.316
350	500.760	704.432	636.080	23.923	544.913	768.521	-114.693
400	571.821	776.008	649.098	50.764	540.226	800.781	-104.569
450	636.222	847.144	667.158	80.994	536.159	833.600	-96.760
500	693.794	917.216	688.672	114.272	532.614	866.870	-90.559
600	790.179	1052.584	738.141	188.665	526.767	934.299	-81.336
700	865.992	1180.313	792.280	271.623	522.392	1002.595	-74.813
800	926.295	1300.035	848.350	361.348	519.338	1071.406	-69.954
900	974.976	1412.046	904.829	456.495	517.433	1140.519	-66.193
1000	1014.813	1516.900	960.850	556.049	516.527	1209.807	-63.193
1100	1047.791	1615.216	1015.916	659.230	516.412	1279.160	-60.741
1200	1075.356	1707.603	1069.747	765.427	516.949	1348.469	-58.696
1300	1098.586	1794.621	1122.192	874.157	517.947	1417.728	-56.964
1400	1118.306	1876.776	1173.184	985.028	519.266	1486.901	-55.476
1500	1135.158	1954.520	1222.705	1097.723	520.832	1555.976	-54.183
1600	1149.646	2028.256	1270.768	1211.981	522.502	1624.928	-53.047
1700	1162.172	2098.338	1317.404	1327.586	524.204	1693.747	-52.041
1800	1173.062	2165.081	1362.658	1444.361	525.854	1762.546	-51.147
1900	1182.575	2228.766	1406.580	1562.153	527.427	1831.188	-50.342
2000	1190.926	2289.641	1449.222	1680.837	528.867	1899.785	-49.616
2100	1198.290	2347.928	1490.640	1800.305	530.083	1968.297	-48.958
2200	1204.811	2403.826	1530.887	1920.467	531.081	2036.756	-48.358
2300	1210.609	2457.512	1570.015	2041.244	531.861	2105.180	-47.809
2400	1215.785	2509.147	1608.077	2162.568	532.338	2173.508	-47.304
2500	1220.420	2558.873	1645.120	2284.382	532.532	2241.969	-46.842
2600	1224.587	2606.822	1681.192	2406.636	532.402	2310.278	-46.413
2700	1228.345	2653.110	1716.337	2529.286	531.956	2378.697	-46.018
2800	1231.744	2697.844	1750.596	2652.294	531.163	2447.158	-45.651
2900	1234.828	2741.122	1784.010	2775.625	529.990	2515.590	-45.310
3000	1237.633	2783.033	1816.616	2899.250	528.496	2584.105	-44.992
3100	1240.193	2823.657	1848.450	3023.143	526.581	2652.570	-44.695
3200	1242.533	2863.069	1879.544	3147.281	524.303	2721.202	-44.418
3300	1244.678	2901.337	1909.930	3271.643	521.641	2789.965	-44.161
3400	1246.649	2938.524	1939.639	3396.211	518.557	2858.694	-43.918
3500	1248.464	2974.688	1968.697	3520.968	515.061	2927.499	-43.690
3600	1250.138	3009.882	1997.132	3645.899	511.185	2996.531	-43.478
3700	1251.686	3044.156	2024.969	3770.991	506.885	3065.686	-43.279
3800	1253.120	3077.556	2052.231	3896.232	502.134	3134.897	-43.091
3900	1254.450	3110.123	2078.941	4021.612	496.981	3204.161	-42.914
4000	1255.687	3141.899	2105.119	4147.119	491.409	3273.749	-42.750
4100	1256.838	3172.920	2130.786	4272.746	485.372	3343.385	-42.594
4200	1257.912	3203.219	2155.961	4398.484	478.906	3413.163	-42.448
4300	1258.915	3232.831	2180.662	4524.326	471.996	3482.983	-42.309
4400	1259.852	3261.783	2204.905	4650.265	464.651	3553.085	-42.180
4500	1260.731	3290.106	2228.707	4776.295	456.892	3623.427	-42.059
4600	1261.555	3317.824	2252.083	4902.409	448.651	3693.968	-41.945
4700	1262.328	3344.964	2275.048	5028.604	439.950	3764.542	-41.837
4800	1263.056	3371.548	2297.616	5154.874	430.843	3835.445	-41.737
4900	1263.741	3397.598	2319.800	5281.214	421.239	3906.363	-41.641
5000	1264.386	3423.136	2341.612	5407.620	411.258	3977.719	-41.554

3.630. Benz[4,10]anthra[1,9,8-*abcd*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 117726-83-7
Point Group: C_s

Length: 15.90 Å
Width: 11.65 Å
Breadth: 3.887 Å
L/B Ratio: 1.364

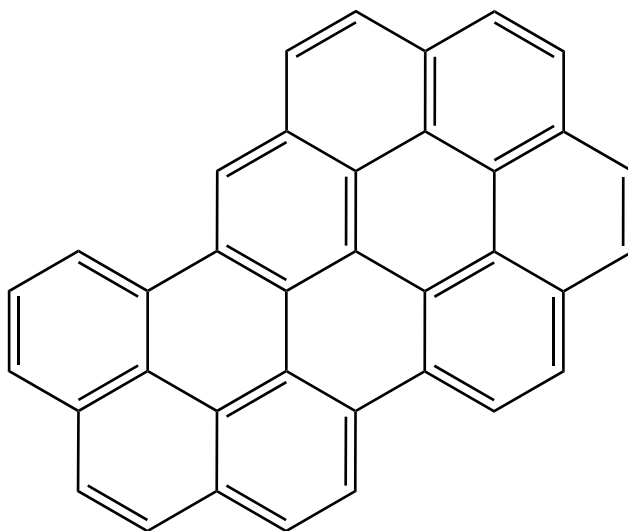
Cartesian coordinates:

C	-0.7871	-3.6747	0.0000	C	-3.2545	-0.2404	0.0000	H	-0.1276	-4.5562	0.0000
C	-2.1420	-3.8163	0.0000	C	0.7359	2.6628	0.0000	H	-2.6014	-4.8113	0.0000
C	-2.9905	-2.6710	0.0000	C	3.5200	2.9540	0.0000	H	-6.3019	-1.7987	0.0000
C	-2.4137	-1.3932	0.0000	C	2.6980	4.0818	0.0000	H	-4.8424	-3.8075	0.0000
C	-5.2106	-1.6965	0.0000	C	1.3253	3.9400	0.0000	H	-1.1074	4.6351	0.0000
C	-4.4080	-2.8012	0.0000	C	1.2494	-2.2328	0.0000	H	-3.5802	4.3659	0.0000
C	-0.9911	-1.2448	0.0000	C	2.1133	-3.3748	0.0000	H	-5.5624	2.9128	0.0000
C	-0.1747	-2.3853	0.0000	C	3.4634	-3.2369	0.0000	H	-6.5639	0.6406	0.0000
C	-0.4108	0.0604	0.0000	C	4.0645	-1.9373	0.0000	H	4.6150	3.0678	0.0000
C	-1.2579	1.2229	0.0000	C	5.4659	-1.7885	0.0000	H	3.1482	5.0800	0.0000
C	-0.7023	2.5058	0.0000	C	6.0269	-0.5298	0.0000	H	0.6701	4.8245	0.0000
C	-1.5648	3.6336	0.0000	C	5.2125	0.6084	0.0000	H	1.6445	-4.3709	0.0000
C	-2.9249	3.4875	0.0000	C	3.2383	-0.7953	0.0000	H	4.1190	-4.1153	0.0000
C	-2.6745	1.0663	0.0000	C	3.8289	0.4951	0.0000	H	6.1009	-2.6816	0.0000
C	-3.5092	2.1948	0.0000	C	2.9720	1.6758	0.0000	H	7.1155	-0.4111	0.0000
C	-4.9267	2.0200	0.0000	C	1.5631	1.5201	0.0000	H	5.6685	1.6105	0.0000
C	-5.4759	0.7738	0.0000	C	0.9758	0.2073	0.0000				
C	-4.6476	-0.3893	0.0000	C	1.8123	-0.9512	0.0000				

Table 3.630: Table of thermodynamic data as a function of temperature for Benz[4,10]anthra[1,9,8-*abcd*]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-59.617	492.935	492.935	∞
100	122.605	371.942	895.014	-52.307	520.048	566.863	-296.093
200	262.223	497.592	664.497	-33.381	505.686	619.417	-161.772
250	341.517	564.578	637.769	-18.298	498.946	648.627	-135.520
298.15	418.279	631.314	631.314	0.000	492.935	678.017	-118.783
300	421.189	633.910	631.322	0.777	492.712	679.162	-118.250
350	497.716	704.642	636.733	23.768	487.155	710.690	-106.062
400	568.784	775.811	649.670	50.456	482.316	742.950	-97.017
450	633.280	846.595	667.625	80.536	478.100	775.788	-90.049
500	690.993	916.363	689.021	113.671	474.410	809.093	-84.524
600	787.707	1051.249	738.248	187.800	468.300	876.633	-76.316
700	863.833	1178.621	792.154	270.527	463.694	945.080	-70.521
800	924.407	1298.073	848.010	360.050	460.437	1014.075	-66.211
900	973.313	1409.875	904.297	455.020	458.356	1083.395	-62.877
1000	1013.340	1514.564	960.146	554.418	457.293	1152.909	-60.221
1100	1046.479	1612.748	1015.058	657.459	457.039	1222.502	-58.051
1200	1074.180	1705.026	1068.749	763.533	457.452	1292.063	-56.241
1300	1097.528	1791.955	1121.070	872.150	458.338	1361.585	-54.708
1400	1117.350	1874.035	1171.949	982.921	459.556	1431.028	-53.391
1500	1134.291	1951.717	1221.367	1095.525	461.032	1500.380	-52.247
1600	1148.857	2025.399	1269.337	1209.700	462.619	1569.616	-51.242
1700	1161.453	2095.435	1315.888	1325.230	464.246	1638.723	-50.351
1800	1172.402	2162.139	1361.064	1441.936	465.827	1707.814	-49.558
1900	1181.970	2225.790	1404.913	1559.665	467.336	1776.752	-48.845
2000	1190.369	2286.635	1447.489	1678.291	468.718	1845.648	-48.202
2100	1197.775	2344.896	1488.846	1797.706	469.881	1914.462	-47.619
2200	1204.335	2400.771	1529.036	1917.818	470.829	1983.225	-47.087
2300	1210.167	2454.437	1568.112	2038.548	471.564	2051.956	-46.600
2400	1215.373	2506.053	1606.124	2159.830	471.997	2120.593	-46.153
2500	1220.037	2555.764	1643.122	2281.605	472.152	2189.363	-45.743
2600	1224.229	2603.697	1679.150	2403.822	471.985	2257.984	-45.363
2700	1228.010	2649.972	1714.255	2526.437	471.504	2326.717	-45.012
2800	1231.430	2694.695	1748.476	2649.412	470.679	2395.492	-44.688
2900	1234.533	2737.962	1781.855	2772.712	469.476	2464.239	-44.385
3000	1237.356	2779.863	1814.427	2896.309	467.952	2533.070	-44.104
3100	1239.931	2820.479	1846.229	3020.175	466.011	2601.853	-43.840
3200	1242.286	2859.883	1877.293	3144.288	463.707	2670.803	-43.595
3300	1244.445	2898.143	1907.651	3268.626	461.021	2739.885	-43.368
3400	1246.428	2935.324	1937.332	3393.171	457.914	2808.934	-43.153
3500	1248.255	2971.481	1966.365	3517.907	454.398	2878.060	-42.952
3600	1249.940	3006.670	1994.776	3642.817	450.501	2947.412	-42.765
3700	1251.498	3040.938	2022.589	3767.890	446.182	3016.889	-42.590
3800	1252.940	3074.333	2049.829	3893.113	441.412	3086.422	-42.425
3900	1254.279	3106.896	2076.518	4018.475	436.242	3156.008	-42.269
4000	1255.524	3138.667	2102.676	4143.966	430.653	3225.919	-42.125
4100	1256.683	3169.684	2128.324	4269.577	424.600	3295.879	-41.989
4200	1257.763	3199.980	2153.480	4395.300	418.119	3365.981	-41.861
4300	1258.772	3229.588	2178.163	4521.127	411.194	3436.124	-41.740
4400	1259.716	3258.537	2202.389	4647.052	403.835	3506.551	-41.627
4500	1260.601	3286.857	2226.175	4773.068	396.064	3577.218	-41.522
4600	1261.430	3314.573	2249.536	4899.170	387.810	3648.084	-41.424
4700	1262.208	3341.710	2272.486	5025.353	379.096	3718.983	-41.331
4800	1262.941	3368.291	2295.039	5151.610	369.978	3790.212	-41.245
4900	1263.630	3394.339	2317.209	5277.939	360.363	3861.455	-41.163
5000	1264.279	3419.875	2339.008	5404.335	350.370	3933.137	-41.088

3.631. Pyreno[1,10,9-*abc*]coronene



Formula: $C_{36}H_{16}$
Mass: 448.512 g/mol
CAS Number: 75459-04-0
Point Group: C_s

Length: 15.93 Å
Width: 11.64 Å
Breadth: 3.886 Å
L/B Ratio: 1.368

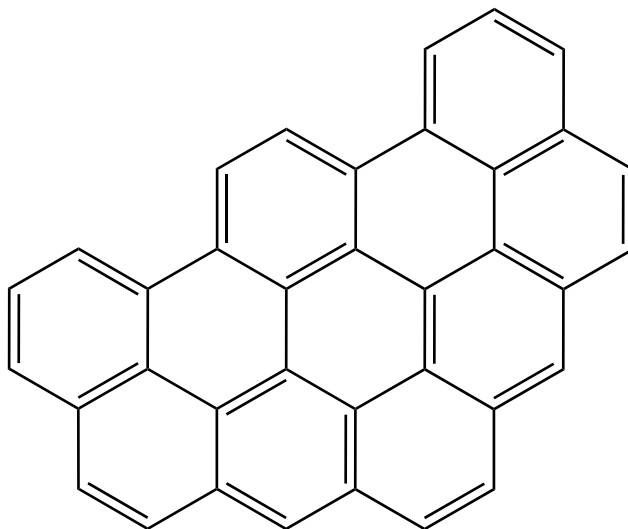
Cartesian coordinates:

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C	-2.5050	-3.6239	0.0000	C	-3.4496	-0.0028	0.0000	H	-3.0053	-4.5990	0.0000
C	-3.2963	-2.4467	0.0000	C	0.9672	-2.1984	0.0000	H	-6.5673	-1.4187	0.0000
C	-2.6603	-1.1954	0.0000	C	1.7727	-3.3646	0.0000	H	-5.2033	-3.4930	0.0000
C	-5.4724	-1.3695	0.0000	C	3.1397	-3.2815	0.0000	H	1.1403	3.6739	0.0000
C	-4.7240	-2.5072	0.0000	C	1.5857	-0.9402	0.0000	H	-1.0689	4.7685	0.0000
C	-1.2374	-1.1154	0.0000	C	1.4256	1.5440	0.0000	H	-3.5462	4.6162	0.0000
C	-0.4749	-2.2885	0.0000	C	0.8007	0.2632	0.0000	H	-5.5977	3.2572	0.0000
C	-0.5974	0.1720	0.0000	C	2.8830	1.6259	0.0000	H	-6.7086	1.0379	0.0000
C	0.6481	2.6878	0.0000	C	5.6896	1.7605	0.0000	H	1.2679	-4.3431	0.0000
C	-1.3847	1.3541	0.0000	C	4.9356	2.9157	0.0000	H	3.7525	-4.1902	0.0000
C	-0.7608	2.6139	0.0000	C	3.5387	2.8506	0.0000	H	6.7843	1.8110	0.0000
C	-1.5706	3.7940	0.0000	C	5.0557	0.5033	0.0000	H	5.4276	3.8941	0.0000
C	-2.9287	3.7106	0.0000	C	3.6482	0.4323	0.0000	H	2.9429	3.7764	0.0000
C	-2.8128	1.2716	0.0000	C	3.0066	-0.8516	0.0000	H	5.7968	-2.8471	0.0000
C	-3.5854	2.4403	0.0000	C	3.7816	-2.0195	0.0000	H	6.9165	-0.6303	0.0000
C	-5.0029	2.3366	0.0000	C	5.2120	-1.9201	0.0000				
C	-5.6151	1.1134	0.0000	C	5.8233	-0.7095	0.0000				

Table 3.631: Table of thermodynamic data as a function of temperature for Pyreno[1,10,9-*abc*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.158	480.645	480.645	∞
100	120.483	365.376	886.241	-52.086	507.978	555.449	-290.131
200	261.174	489.844	656.467	-33.325	493.452	608.733	-158.981
250	340.980	556.654	629.775	-18.280	486.672	638.335	-133.370
298.15	418.064	623.325	623.325	0.000	480.645	668.108	-117.047
300	420.984	625.920	623.333	0.776	480.421	669.268	-116.528
350	497.698	696.635	628.742	23.763	474.859	701.196	-104.646
400	568.865	767.809	641.677	50.453	470.021	733.856	-95.830
450	633.410	838.606	659.632	80.538	465.811	767.094	-89.040
500	691.150	908.389	681.029	113.680	462.129	800.798	-83.657
600	787.892	1043.307	730.262	187.827	456.035	869.134	-75.663
700	864.043	1170.709	784.177	270.573	451.449	938.374	-70.021
800	924.641	1290.191	840.043	360.118	448.215	1008.158	-65.825
900	973.567	1402.022	896.341	455.113	446.158	1078.265	-62.580
1000	1013.607	1506.738	952.201	554.536	445.121	1148.563	-59.994
1100	1046.752	1604.948	1007.125	657.605	444.894	1218.938	-57.881
1200	1074.454	1697.250	1060.828	763.706	445.334	1289.278	-56.120
1300	1097.798	1784.200	1113.161	872.351	446.248	1359.576	-54.627
1400	1117.613	1866.300	1164.052	983.148	447.493	1429.794	-53.345
1500	1134.544	1944.000	1213.482	1095.778	448.994	1499.918	-52.231
1600	1149.099	2017.698	1261.462	1209.978	450.606	1569.925	-51.252
1700	1161.683	2087.748	1308.024	1325.532	452.256	1639.801	-50.384
1800	1172.621	2154.465	1353.210	1442.259	453.860	1709.660	-49.612
1900	1182.176	2218.127	1397.069	1560.010	455.390	1779.365	-48.917
2000	1190.564	2278.983	1439.655	1678.656	456.792	1849.027	-48.291
2100	1197.959	2337.253	1481.020	1798.090	457.974	1918.606	-47.722
2200	1204.508	2393.136	1521.219	1918.219	458.940	1988.133	-47.203
2300	1210.331	2446.810	1560.303	2038.967	459.692	2057.626	-46.729
2400	1215.528	2498.433	1598.323	2160.265	460.141	2127.025	-46.293
2500	1220.183	2548.149	1635.328	2282.054	460.311	2196.558	-45.894
2600	1224.367	2596.089	1671.364	2404.286	460.158	2265.939	-45.522
2700	1228.140	2642.369	1706.475	2526.914	459.691	2335.433	-45.181
2800	1231.553	2687.096	1740.703	2649.902	458.878	2404.968	-44.864
2900	1234.650	2730.368	1774.087	2773.214	457.687	2474.475	-44.569
3000	1237.467	2772.272	1806.665	2896.822	456.175	2544.065	-44.295
3100	1240.036	2812.891	1838.472	3020.699	454.244	2613.607	-44.038
3200	1242.386	2852.299	1869.542	3144.822	451.951	2683.316	-43.800
3300	1244.539	2890.562	1899.905	3269.170	449.275	2753.156	-43.578
3400	1246.518	2927.745	1929.591	3393.724	446.177	2822.963	-43.369
3500	1248.340	2963.905	1958.629	3518.468	442.669	2892.846	-43.172
3600	1250.021	2999.096	1987.044	3643.388	438.780	2962.956	-42.990
3700	1251.575	3033.367	2014.862	3768.468	434.469	3033.191	-42.820
3800	1253.015	3066.764	2042.106	3893.699	429.707	3103.481	-42.659
3900	1254.350	3099.329	2068.798	4019.068	424.545	3173.824	-42.508
4000	1255.592	3131.102	2094.960	4144.566	418.962	3244.491	-42.368
4100	1256.748	3162.120	2120.612	4270.183	412.916	3315.207	-42.235
4200	1257.826	3192.418	2145.772	4395.913	406.441	3386.065	-42.111
4300	1258.832	3222.027	2170.458	4521.746	399.523	3456.965	-41.993
4400	1259.774	3250.978	2194.688	4647.677	392.170	3528.147	-41.884
4500	1260.656	3279.298	2218.476	4773.699	384.404	3599.570	-41.782
4600	1261.483	3307.015	2241.840	4899.806	376.155	3671.193	-41.687
4700	1262.259	3334.154	2264.793	5025.994	367.446	3742.847	-41.596
4800	1262.989	3360.736	2287.349	5152.257	358.333	3814.832	-41.513
4900	1263.677	3386.785	2309.522	5278.590	348.723	3886.830	-41.433
5000	1264.325	3412.322	2331.323	5404.991	338.735	3959.268	-41.361

3.632. Dinaphtho[8,1,2-*abc*:2',1',8'-*klm*]coronene



Formula: $C_{36}H_{16}$
Mass: 448.512 g/mol
CAS Number: 53086-28-5
Point Group: C_{2v}

Length: 15.94 Å
Width: 11.65 Å
Breadth: 3.891 Å
L/B Ratio: 1.369

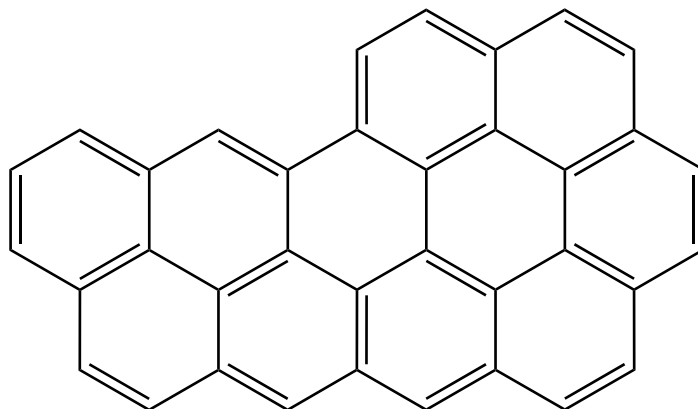
Cartesian coordinates:

C	0.6661	-3.1345	0.0000	C	-5.0154	-3.0422	0.0000	H	1.2194	-4.0866	0.0000
C	-0.7137	-3.1241	0.0000	C	-3.6238	-3.0780	0.0000	H	-1.2814	-4.0676	0.0000
C	-1.4260	-1.9137	0.0000	C	-2.8256	0.5762	0.0000	H	3.3947	3.9148	0.0000
C	-0.7135	-0.7013	0.0000	C	-3.5142	1.8113	0.0000	H	1.2786	5.1549	0.0000
C	0.7028	-0.7120	0.0000	C	-4.9552	1.8056	0.0000	H	-1.2001	5.1737	0.0000
C	1.3967	-1.9351	0.0000	C	-5.6484	0.6444	0.0000	H	-3.3348	3.9659	0.0000
C	1.4255	0.5346	0.0000	C	-4.9714	-0.6274	0.0000	H	-6.7846	-1.8082	0.0000
C	2.8419	2.9672	0.0000	C	-3.5603	-0.6570	0.0000	H	-5.5798	-3.9806	0.0000
C	0.7311	1.7597	0.0000	C	2.8509	-1.9408	0.0000	H	-3.0903	-4.0411	0.0000
C	1.4458	2.9800	0.0000	C	3.5766	-3.1327	0.0000	H	-5.4730	2.7717	0.0000
C	0.7083	4.2187	0.0000	C	4.9685	-3.1181	0.0000	H	-6.7446	0.6421	0.0000
C	-0.6440	4.2290	0.0000	C	5.6605	-1.9170	0.0000	H	3.0285	-4.0876	0.0000
C	-0.7042	1.7706	0.0000	C	2.8341	0.5332	0.0000	H	5.5186	-4.0650	0.0000
C	-1.4003	3.0016	0.0000	C	3.5499	-0.7110	0.0000	H	6.7563	-1.9111	0.0000
C	-2.7965	3.0100	0.0000	C	4.9613	-0.7029	0.0000	H	6.7536	0.5395	0.0000
C	-1.4172	0.5562	0.0000	C	5.6576	0.5584	0.0000	H	5.5146	2.6882	0.0000
C	-2.8801	-1.8973	0.0000	C	4.9821	1.7301	0.0000				
C	-5.6889	-1.8307	0.0000	C	3.5414	1.7577	0.0000				

Table 3.632: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*abc*:2',1',8'-*klm*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.235	493.638	493.638	∞
100	120.456	357.475	879.649	-52.217	520.840	569.102	-297.262
200	261.908	482.220	649.276	-33.411	506.359	623.164	-162.750
250	341.871	549.211	622.515	-18.326	499.620	653.143	-136.464
298.15	419.071	616.049	616.049	0.000	493.638	683.270	-119.704
300	421.994	618.651	616.057	0.778	493.416	684.444	-119.170
350	498.786	689.528	621.480	23.817	487.907	716.731	-106.964
400	569.985	760.850	634.443	50.563	483.125	749.743	-97.904
450	634.524	831.778	652.436	80.704	478.970	783.325	-90.924
500	692.231	901.678	673.876	113.901	475.343	817.368	-85.388
600	788.870	1036.783	723.199	188.151	469.353	886.365	-77.163
700	864.904	1164.328	777.202	270.988	464.858	956.250	-71.355
800	925.394	1283.917	833.149	360.615	461.705	1026.667	-67.033
900	974.226	1395.831	889.520	455.680	459.718	1097.397	-63.690
1000	1014.186	1500.613	945.448	555.165	458.743	1168.310	-61.025
1100	1047.263	1598.874	1000.431	658.288	458.570	1239.295	-58.848
1200	1074.907	1691.219	1054.188	764.437	459.059	1310.240	-57.032
1300	1098.202	1778.203	1106.568	873.125	460.015	1381.139	-55.494
1400	1117.975	1860.332	1157.503	983.960	461.298	1451.955	-54.172
1500	1134.870	1938.055	1206.972	1096.624	462.834	1522.675	-53.023
1600	1149.393	2011.773	1254.988	1210.855	464.477	1593.275	-52.014
1700	1161.950	2081.840	1301.583	1326.437	466.155	1663.743	-51.120
1800	1172.864	2148.572	1346.799	1443.191	467.784	1734.193	-50.324
1900	1182.399	2212.246	1390.686	1560.964	469.338	1804.486	-49.608
2000	1190.768	2273.113	1433.297	1679.631	470.761	1874.736	-48.962
2100	1198.147	2331.393	1474.686	1799.085	471.963	1944.901	-48.376
2200	1204.681	2387.285	1514.906	1919.233	472.947	2015.013	-47.842
2300	1210.491	2440.965	1554.010	2039.997	473.715	2085.092	-47.353
2400	1215.676	2492.595	1592.049	2161.310	474.180	2155.075	-46.903
2500	1220.321	2542.317	1629.072	2283.114	474.364	2225.191	-46.492
2600	1224.496	2590.262	1665.124	2405.359	474.225	2295.156	-46.109
2700	1228.260	2636.547	1700.250	2528.000	473.770	2365.232	-45.757
2800	1231.666	2681.278	1734.493	2650.999	472.969	2435.349	-45.431
2900	1234.755	2724.554	1767.891	2774.322	471.788	2505.438	-45.127
3000	1237.566	2766.462	1800.482	2897.941	470.286	2575.609	-44.844
3100	1240.129	2807.084	1832.301	3021.827	468.365	2645.731	-44.579
3200	1242.474	2846.494	1863.382	3145.959	466.081	2716.021	-44.334
3300	1244.623	2884.760	1893.755	3270.315	463.413	2786.441	-44.105
3400	1246.597	2921.946	1923.452	3394.878	460.324	2856.829	-43.889
3500	1248.415	2958.108	1952.499	3519.630	456.823	2927.292	-43.687
3600	1250.092	2993.301	1980.924	3644.556	452.942	2997.981	-43.499
3700	1251.642	3027.573	2008.751	3769.644	448.638	3068.795	-43.323
3800	1253.078	3060.972	2036.003	3894.881	443.883	3139.664	-43.157
3900	1254.411	3093.539	2062.704	4020.256	438.726	3210.586	-43.000
4000	1255.650	3125.313	2088.873	4145.760	433.150	3281.833	-42.855
4100	1256.803	3156.333	2114.532	4271.383	427.109	3353.128	-42.718
4200	1257.878	3186.632	2139.699	4397.118	420.640	3424.564	-42.590
4300	1258.882	3216.242	2164.392	4522.956	413.726	3496.043	-42.468
4400	1259.822	3245.194	2188.628	4648.892	406.378	3567.804	-42.354
4500	1260.702	3273.516	2212.423	4774.919	398.617	3639.805	-42.249
4600	1261.527	3301.234	2235.792	4901.031	390.372	3712.005	-42.150
4700	1262.302	3328.373	2258.751	5027.222	381.668	3784.238	-42.056
4800	1263.030	3354.956	2281.313	5153.489	372.559	3856.800	-41.970
4900	1263.716	3381.006	2303.491	5279.827	362.953	3929.377	-41.887
5000	1264.362	3406.543	2325.297	5406.231	352.969	4002.392	-41.812

3.633. Pyreno[10,1,2-*abc*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 75449-90-0
Point Group: C_s

Length: 16.55 Å
Width: 11.67 Å
Breadth: 3.887 Å
L/B Ratio: 1.417

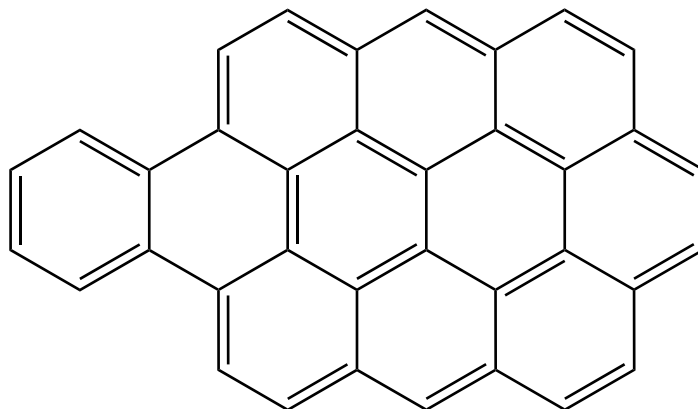
Cartesian coordinates:

C	-0.4610	-3.2595	0.0000	C	-4.7695	1.1369	0.0000	H	-0.3129	-4.3466	0.0000
C	-1.7506	-2.7363	0.0000	C	-3.4676	0.6116	0.0000	H	-5.0411	-3.7318	0.0000
C	-1.9409	-1.3298	0.0000	C	1.4324	1.2891	0.0000	H	-2.7477	-4.6755	0.0000
C	-4.1626	-3.0763	0.0000	C	2.5367	2.1088	0.0000	H	-6.8872	0.6701	0.0000
C	-2.9098	-3.5914	0.0000	C	1.6058	-0.1357	0.0000	H	-6.5439	-1.7874	0.0000
C	-4.3796	-1.6551	0.0000	C	0.4730	-1.0049	0.0000	H	0.7306	3.8906	0.0000
C	-3.2732	-0.7959	0.0000	C	0.6574	-2.4105	0.0000	H	-1.5768	4.8257	0.0000
C	-5.8740	0.2522	0.0000	C	1.9827	-2.9404	0.0000	H	-4.0161	4.4836	0.0000
C	-5.6839	-1.1078	0.0000	C	3.8538	1.5740	0.0000	H	-5.9708	2.9533	0.0000
C	-0.8328	-0.4685	0.0000	C	6.4390	0.4749	0.0000	H	2.4006	3.2025	0.0000
C	-1.0192	0.9629	0.0000	C	6.2559	1.8665	0.0000	H	2.1132	-4.0297	0.0000
C	0.0789	1.8303	0.0000	C	4.9920	2.4120	0.0000	H	7.4542	0.0624	0.0000
C	-0.1455	3.2234	0.0000	C	2.8936	-0.6826	0.0000	H	7.1350	2.5197	0.0000
C	-1.4200	3.7410	0.0000	C	3.0727	-2.1084	0.0000	H	4.8545	3.4991	0.0000
C	-2.3369	1.4911	0.0000	C	4.4247	-2.6309	0.0000	H	4.5466	-3.7204	0.0000
C	-2.5397	2.8832	0.0000	C	5.4960	-1.8136	0.0000	H	6.5153	-2.2169	0.0000
C	-3.8785	3.3962	0.0000	C	5.3443	-0.3737	0.0000				
C	-4.9481	2.5590	0.0000	C	4.0318	0.1737	0.0000				

Table 3.633: Table of thermodynamic data as a function of temperature for Pyreno[10,1,2-*abc*]coronene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-59.612	505.757	505.757	∞
100	121.317	367.856	892.577	-52.472	532.705	579.928	-302.917
200	263.227	493.273	661.104	-33.566	518.323	632.918	-165.298
250	343.480	560.593	634.221	-18.407	511.658	662.336	-138.385
298.15	420.804	627.727	627.727	0.000	505.757	691.908	-121.217
300	423.729	630.339	627.735	0.781	505.538	693.060	-120.670
350	500.522	701.486	633.179	23.907	500.117	724.756	-108.162
400	571.651	773.035	646.190	50.738	495.420	757.164	-98.873
450	636.087	844.154	664.242	80.961	491.346	790.132	-91.714
500	693.682	914.212	685.747	114.233	487.794	823.552	-86.034
600	790.109	1049.563	735.202	188.617	481.938	891.282	-77.591
700	865.969	1177.285	789.329	271.570	477.559	959.880	-71.626
800	926.320	1297.008	845.389	361.295	474.504	1028.994	-67.185
900	975.041	1409.024	901.861	456.447	472.604	1098.410	-63.749
1000	1014.911	1513.887	957.877	556.009	471.707	1168.000	-61.009
1100	1047.913	1612.214	1012.940	659.201	471.602	1237.653	-58.770
1200	1075.492	1704.612	1066.769	765.411	472.153	1307.262	-56.902
1300	1098.731	1791.640	1119.214	874.155	473.164	1376.820	-55.320
1400	1118.455	1873.806	1170.206	985.041	474.498	1446.290	-53.961
1500	1135.307	1951.561	1219.728	1097.750	476.080	1515.661	-52.779
1600	1149.793	2025.306	1267.792	1212.023	477.764	1584.909	-51.741
1700	1162.316	2095.397	1314.430	1327.644	479.481	1654.023	-50.821
1800	1173.200	2162.148	1359.686	1444.432	481.145	1723.116	-50.002
1900	1182.708	2225.840	1403.610	1562.238	482.731	1792.051	-49.266
2000	1191.053	2286.722	1446.255	1680.935	484.184	1860.940	-48.602
2100	1198.411	2345.016	1487.675	1800.415	485.413	1929.743	-47.999
2200	1204.926	2400.919	1527.924	1920.589	486.422	1998.493	-47.449
2300	1210.719	2454.611	1567.055	2041.377	487.214	2067.207	-46.947
2400	1215.888	2506.250	1605.120	2162.712	487.701	2135.826	-46.484
2500	1220.519	2555.980	1642.166	2284.536	487.906	2204.575	-46.061
2600	1224.681	2603.932	1678.240	2406.800	487.785	2273.174	-45.668
2700	1228.434	2650.224	1713.387	2529.459	487.348	2341.882	-45.305
2800	1231.828	2694.961	1747.649	2652.475	486.564	2410.631	-44.970
2900	1234.908	2738.242	1781.065	2775.814	485.399	2479.351	-44.657
3000	1237.710	2780.156	1813.673	2899.447	483.913	2548.154	-44.366
3100	1240.265	2820.782	1845.509	3023.348	482.005	2616.906	-44.094
3200	1242.602	2860.196	1876.605	3147.493	479.734	2685.826	-43.841
3300	1244.744	2898.467	1906.993	3271.862	477.079	2754.876	-43.605
3400	1246.712	2935.656	1936.704	3396.436	474.001	2823.892	-43.383
3500	1248.524	2971.821	1965.764	3521.199	470.512	2892.984	-43.175
3600	1250.195	3007.017	1994.201	3646.136	466.641	2962.302	-42.981
3700	1251.741	3041.292	2022.040	3771.234	462.347	3031.744	-42.800
3800	1253.172	3074.693	2049.304	3896.480	457.602	3101.242	-42.629
3900	1254.500	3107.262	2076.015	4021.865	452.454	3170.791	-42.467
4000	1255.735	3139.039	2102.195	4147.377	446.886	3240.665	-42.318
4100	1256.884	3170.061	2127.864	4273.009	440.854	3310.588	-42.177
4200	1257.956	3200.362	2153.040	4398.751	434.393	3380.651	-42.044
4300	1258.957	3229.974	2177.742	4524.598	427.487	3450.757	-41.918
4400	1259.893	3258.928	2201.987	4650.541	420.146	3521.144	-41.800
4500	1260.770	3287.251	2225.790	4776.574	412.391	3591.772	-41.691
4600	1261.592	3314.970	2249.168	4902.693	404.154	3662.599	-41.589
4700	1262.364	3342.111	2272.134	5028.891	395.456	3733.458	-41.492
4800	1263.090	3368.696	2294.703	5155.164	386.353	3804.646	-41.402
4900	1263.774	3394.747	2316.888	5281.507	376.753	3875.849	-41.316
5000	1264.418	3420.285	2338.701	5407.917	366.775	3947.490	-41.238

3.634. Benz[*d*]ovalene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 75449-89-7
Point Group: C_{2v}

Length: 16.53 Å
Width: 11.66 Å
Breadth: 3.890 Å
L/B Ratio: 1.418

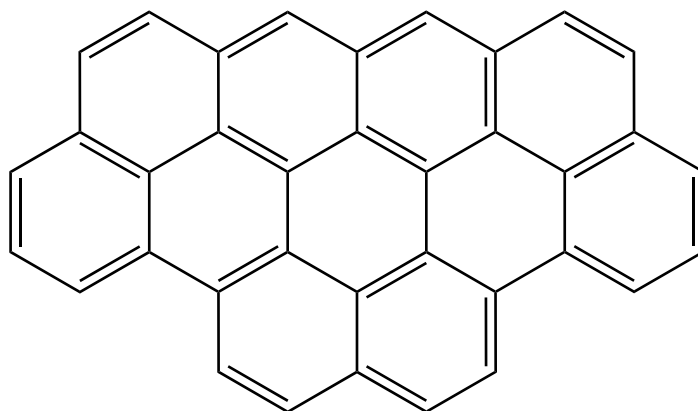
Cartesian coordinates:

C	0.7849	3.5298	0.0000	C	-2.9044	1.4349	0.0000	H	0.7863	4.6268	0.0000
C	1.9894	2.8348	0.0000	C	-1.7048	0.7247	0.0000	H	5.3880	3.3571	0.0000
C	1.9823	1.4148	0.0000	C	-0.4566	1.4280	0.0000	H	3.2510	4.6138	0.0000
C	4.4261	2.8315	0.0000	C	-0.4399	2.8418	0.0000	H	0.7504	-4.6328	0.0000
C	3.2589	3.5176	0.0000	C	-1.6877	3.5426	0.0000	H	3.2151	-4.6388	0.0000
C	0.7641	0.7171	0.0000	C	-2.8661	2.8646	0.0000	H	5.3618	-3.3988	0.0000
C	0.7585	-0.7229	0.0000	C	-1.7104	-0.7114	0.0000	H	6.5921	-1.2657	0.0000
C	0.7575	-3.5358	0.0000	C	-2.9155	-1.4123	0.0000	H	6.6017	1.2144	0.0000
C	1.9713	-1.4301	0.0000	C	-2.8882	-2.8422	0.0000	H	-1.6714	4.6385	0.0000
C	1.9673	-2.8501	0.0000	C	-1.7152	-3.5294	0.0000	H	-3.8271	3.4017	0.0000
C	3.2315	-3.5428	0.0000	C	-0.4619	-2.8383	0.0000	H	-3.8534	-3.3719	0.0000
C	4.4040	-2.8658	0.0000	C	-0.4677	-1.4244	0.0000	H	-1.7073	-4.6254	0.0000
C	4.4438	1.3922	0.0000	C	-4.1610	-0.6882	0.0000	H	-5.3732	2.5125	0.0000
C	3.2232	0.6966	0.0000	C	-4.1556	0.7205	0.0000	H	-7.5323	1.2723	0.0000
C	3.2177	-0.7216	0.0000	C	-5.3904	1.4118	0.0000	H	-7.5419	-1.2138	0.0000
C	4.4328	-1.4267	0.0000	C	-6.5818	0.7288	0.0000	H	-5.3925	-2.4707	0.0000
C	5.6465	-0.7112	0.0000	C	-6.5873	-0.6777	0.0000				
C	5.6519	0.6673	0.0000	C	-5.4012	-1.3699	0.0000				

Table 3.634: Table of thermodynamic data as a function of temperature for Benz[*d*]ovalene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-59.222	495.988	495.988	∞
100	120.510	357.069	879.085	-52.202	523.207	571.509	-298.519
200	261.847	481.791	648.787	-33.399	508.721	625.612	-163.390
250	341.754	548.764	622.037	-18.318	501.978	655.613	-136.980
298.15	418.858	615.574	615.574	0.000	495.988	685.763	-120.140
300	421.777	618.174	615.582	0.778	495.766	686.937	-119.604
350	498.465	689.010	621.001	23.803	490.243	719.249	-107.340
400	569.580	760.283	633.957	50.531	485.443	752.288	-98.237
450	634.064	831.160	651.938	80.650	481.266	785.900	-91.223
500	691.741	901.009	673.363	113.823	477.615	819.975	-85.660
600	788.370	1036.024	722.652	188.023	471.575	889.043	-77.396
700	864.428	1163.493	776.619	270.812	467.032	959.008	-71.561
800	924.953	1283.021	832.531	360.392	463.833	1029.512	-67.219
900	973.823	1394.886	888.869	455.415	461.804	1100.334	-63.860
1000	1013.819	1499.626	944.764	554.862	460.790	1171.344	-61.183
1100	1046.930	1597.855	999.718	657.950	460.582	1242.429	-58.997
1200	1074.604	1690.171	1053.449	764.067	461.039	1313.477	-57.173
1300	1097.926	1777.132	1105.804	872.726	461.966	1384.482	-55.628
1400	1117.723	1859.241	1156.716	983.535	463.223	1455.407	-54.301
1500	1134.640	1936.948	1206.165	1096.175	464.735	1526.237	-53.147
1600	1149.183	2010.652	1254.162	1210.384	466.356	1596.948	-52.134
1700	1161.757	2080.707	1300.739	1325.946	468.014	1667.529	-51.236
1800	1172.686	2147.428	1345.939	1442.681	469.625	1738.092	-50.437
1900	1182.235	2211.093	1389.811	1560.437	471.162	1808.501	-49.718
2000	1190.617	2271.952	1432.407	1679.089	472.569	1878.866	-49.070
2100	1198.007	2330.225	1473.783	1798.528	473.756	1949.147	-48.481
2200	1204.552	2386.110	1513.991	1918.662	474.726	2019.377	-47.945
2300	1210.370	2439.785	1553.084	2039.414	475.482	2089.573	-47.455
2400	1215.564	2491.410	1591.112	2160.715	475.936	2159.675	-47.003
2500	1220.216	2541.128	1628.124	2282.508	476.109	2229.909	-46.590
2600	1224.398	2589.068	1664.167	2404.743	475.959	2299.993	-46.206
2700	1228.168	2635.350	1699.285	2527.374	475.495	2370.188	-45.853
2800	1231.579	2680.078	1733.519	2650.365	474.685	2440.425	-45.526
2900	1234.674	2723.350	1766.909	2773.680	473.496	2510.635	-45.220
3000	1237.489	2765.256	1799.493	2897.290	471.986	2580.926	-44.937
3100	1240.057	2805.876	1831.305	3021.169	470.058	2651.169	-44.671
3200	1242.406	2845.283	1862.379	3145.294	467.766	2721.580	-44.424
3300	1244.558	2883.548	1892.746	3269.644	465.092	2792.121	-44.195
3400	1246.536	2920.731	1922.437	3394.200	461.996	2862.630	-43.978
3500	1248.357	2956.892	1951.479	3518.946	458.490	2933.215	-43.775
3600	1250.037	2992.083	1979.898	3643.867	454.603	3004.026	-43.586
3700	1251.590	3026.354	2007.719	3768.949	450.293	3074.962	-43.410
3800	1253.029	3059.751	2034.967	3894.181	445.533	3145.953	-43.243
3900	1254.364	3092.317	2061.663	4019.551	440.372	3216.997	-43.086
4000	1255.604	3124.090	2087.828	4145.050	434.791	3288.366	-42.941
4100	1256.760	3155.109	2113.482	4270.669	428.746	3359.783	-42.803
4200	1257.837	3185.407	2138.645	4396.400	422.272	3431.342	-42.674
4300	1258.843	3215.016	2163.334	4522.234	415.355	3502.943	-42.551
4400	1259.784	3243.967	2187.566	4648.166	408.002	3574.826	-42.438
4500	1260.665	3272.288	2211.357	4774.189	400.237	3646.951	-42.332
4600	1261.492	3300.005	2234.723	4900.297	391.990	3719.274	-42.233
4700	1262.268	3327.144	2257.679	5026.486	383.282	3791.630	-42.138
4800	1262.998	3353.726	2280.237	5152.750	374.170	3864.315	-42.051
4900	1263.685	3379.776	2302.412	5279.084	364.560	3937.014	-41.968
5000	1264.333	3405.312	2324.215	5405.485	354.574	4010.153	-41.893

3.635. Dinaphtho[8,1,2-*abc*:2',1',8'-*hij*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128345-74-4
Point Group: C_{2v}

Length: 16.56 Å
Width: 11.68 Å
Breadth: 3.885 Å
L/B Ratio: 1.418

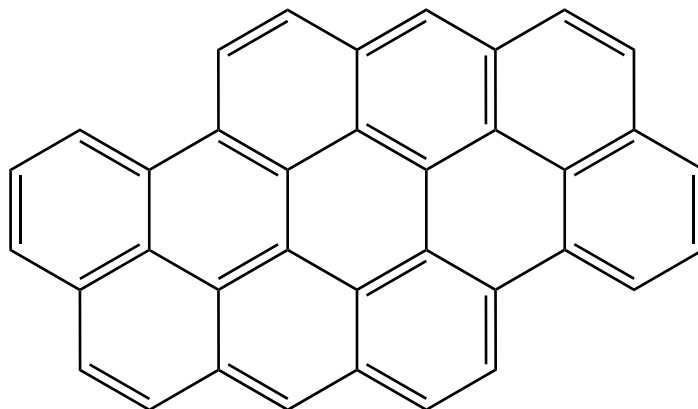
Cartesian coordinates:

C	1.2435	-3.1682	0.0000	C	-6.1261	0.9986	0.0000	H	1.2380	-4.2653	0.0000
C	0.0077	-2.4756	0.0000	C	-6.1128	-0.3948	0.0000	H	-1.2117	-4.2729	0.0000
C	0.0033	-1.0611	0.0000	C	-3.6840	-0.3597	0.0000	H	3.3737	3.7508	0.0000
C	-1.2238	-3.1758	0.0000	C	-4.9010	-1.0828	0.0000	H	1.2142	4.9941	0.0000
C	1.2342	-0.3505	0.0000	C	-4.8604	-2.5278	0.0000	H	-1.2451	4.9865	0.0000
C	1.2364	1.0882	0.0000	C	-3.6888	-3.1963	0.0000	H	-3.3969	3.7298	0.0000
C	2.4410	1.7949	0.0000	C	-2.4240	-2.4945	0.0000	H	-4.9494	2.8150	0.0000
C	2.4111	3.2162	0.0000	C	-2.4366	-1.0665	0.0000	H	-7.0831	1.5310	0.0000
C	1.2276	3.8982	0.0000	C	3.6970	1.0753	0.0000	H	-7.0567	-0.9516	0.0000
C	-0.0055	1.7921	0.0000	C	6.1151	-0.3570	0.0000	H	-5.8164	-3.0641	0.0000
C	-0.0099	3.1982	0.0000	C	6.1198	1.0364	0.0000	H	-3.6638	-4.2922	0.0000
C	-1.2517	3.8905	0.0000	C	4.9300	1.7447	0.0000	H	7.0625	-0.9078	0.0000
C	-2.4309	3.2012	0.0000	C	4.9076	-1.0525	0.0000	H	7.0736	1.5746	0.0000
C	-1.2431	1.0806	0.0000	C	3.6862	-0.3368	0.0000	H	4.9318	2.8456	0.0000
C	-2.4521	1.7797	0.0000	C	2.4432	-1.0514	0.0000	H	3.6902	-4.2694	0.0000
C	-1.2320	-0.3582	0.0000	C	2.4394	-2.4794	0.0000	H	5.8352	-3.0281	0.0000
C	-3.7036	1.0524	0.0000	C	3.7085	-3.1734	0.0000				
C	-4.9406	1.7142	0.0000	C	4.8759	-2.4977	0.0000				

Table 3.635: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*abc*:2',1',8'-*hij*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.227	504.188	504.188	∞
100	120.476	356.950	879.205	-52.226	531.382	579.696	-302.796
200	261.969	481.729	648.800	-33.414	516.905	633.809	-165.531
250	341.907	548.733	622.038	-18.326	510.169	663.812	-138.693
298.15	419.041	615.572	615.572	0.000	504.188	693.962	-121.577
300	421.961	618.173	615.580	0.778	503.966	695.137	-121.032
350	498.668	689.039	621.002	23.813	498.453	727.448	-108.563
400	569.790	760.340	633.963	50.551	493.663	760.485	-99.307
450	634.272	831.242	651.951	80.681	489.497	794.094	-92.174
500	691.940	901.113	673.384	113.864	485.856	828.164	-86.516
600	788.545	1036.162	722.690	188.083	479.835	897.220	-78.108
700	864.578	1163.656	776.673	270.888	475.308	967.170	-72.170
800	925.080	1283.202	832.599	360.482	472.122	1037.656	-67.751
900	973.932	1395.081	888.951	455.517	470.105	1108.460	-64.332
1000	1013.913	1499.832	944.858	554.974	469.101	1179.450	-61.607
1100	1047.011	1598.069	999.823	658.071	468.902	1250.513	-59.381
1200	1074.676	1690.392	1053.562	764.195	469.367	1321.540	-57.524
1300	1097.989	1777.358	1105.927	872.861	470.301	1392.523	-55.951
1400	1117.779	1859.472	1156.846	983.676	471.564	1463.425	-54.600
1500	1134.690	1937.182	1206.302	1096.321	473.081	1534.231	-53.426
1600	1149.228	2010.889	1254.305	1210.535	474.707	1604.919	-52.394
1700	1161.798	2080.947	1300.887	1326.101	476.369	1675.476	-51.480
1800	1172.724	2147.670	1346.092	1442.840	477.983	1746.015	-50.667
1900	1182.269	2211.337	1389.969	1560.600	479.524	1816.399	-49.935
2000	1190.648	2272.197	1432.570	1679.255	480.934	1886.740	-49.276
2100	1198.036	2330.472	1473.949	1798.697	482.124	1956.997	-48.677
2200	1204.578	2386.358	1514.161	1918.834	483.097	2027.202	-48.131
2300	1210.395	2440.035	1553.257	2039.588	483.856	2097.373	-47.632
2400	1215.587	2491.660	1591.289	2160.892	484.312	2167.450	-47.172
2500	1220.237	2541.379	1628.304	2282.687	484.487	2237.659	-46.752
2600	1224.417	2589.321	1664.350	2404.924	484.339	2307.718	-46.362
2700	1228.187	2635.602	1699.470	2527.557	483.877	2377.888	-46.002
2800	1231.597	2680.331	1733.707	2650.549	483.069	2448.100	-45.669
2900	1234.690	2723.604	1767.099	2773.866	481.881	2518.283	-45.358
3000	1237.504	2765.511	1799.685	2897.478	480.373	2588.550	-45.070
3100	1240.071	2806.131	1831.499	3021.358	478.446	2658.767	-44.799
3200	1242.419	2845.539	1862.575	3145.485	476.156	2729.152	-44.548
3300	1244.571	2883.804	1892.944	3269.836	473.483	2799.668	-44.314
3400	1246.548	2920.987	1922.637	3394.393	470.389	2870.151	-44.094
3500	1248.368	2957.148	1951.680	3519.140	466.884	2940.710	-43.887
3600	1250.048	2992.340	1980.100	3644.062	462.998	3011.496	-43.695
3700	1251.600	3026.611	2007.923	3769.145	458.689	3082.406	-43.515
3800	1253.038	3060.009	2035.172	3894.378	453.930	3153.371	-43.345
3900	1254.373	3092.574	2061.869	4019.750	448.769	3224.390	-43.185
4000	1255.613	3124.348	2088.036	4145.250	443.189	3295.732	-43.037
4100	1256.768	3155.367	2113.691	4270.869	437.145	3367.124	-42.897
4200	1257.845	3185.665	2138.855	4396.601	430.672	3438.658	-42.765
4300	1258.851	3215.275	2163.545	4522.436	423.756	3510.233	-42.640
4400	1259.791	3244.226	2187.779	4648.369	416.404	3582.090	-42.524
4500	1260.672	3272.547	2211.571	4774.392	408.640	3654.188	-42.416
4600	1261.499	3300.264	2234.938	4900.501	400.393	3726.486	-42.315
4700	1262.275	3327.403	2257.894	5026.690	391.686	3798.816	-42.218
4800	1263.004	3353.986	2280.454	5152.955	382.574	3871.475	-42.129
4900	1263.691	3380.035	2302.629	5279.290	372.965	3944.149	-42.044
5000	1264.338	3405.572	2324.433	5405.691	362.979	4017.261	-41.967

3.636. Dinaphtho[8,1,2-*abc*:8',1',2'-*jkl*]coronene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 190-47-6
Point Group: C_{2h}

Length: 16.55 Å
Width: 11.67 Å
Breadth: 3.886 Å
L/B Ratio: 1.418

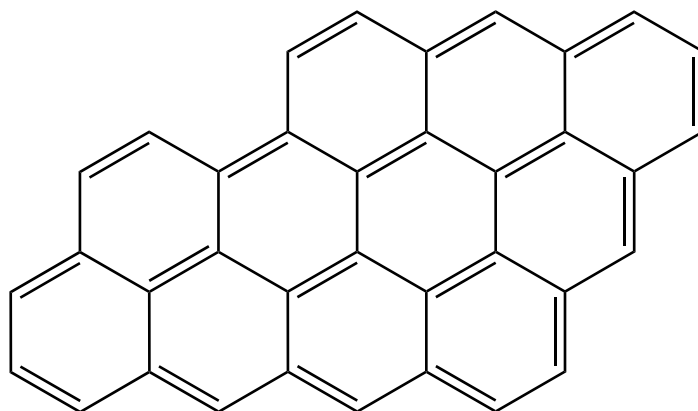
Cartesian coordinates:

C	1.8330	-3.2550	0.0000	C	-5.8863	1.8076	0.0000	H	2.6798	-3.9590	0.0000
C	0.5459	-3.7035	0.0000	C	-6.1432	0.4389	0.0000	H	0.3277	-4.7776	0.0000
C	-0.5454	-2.7846	0.0000	C	-3.7534	0.0019	0.0000	H	-2.0830	-4.3146	0.0000
C	-0.2725	-1.4002	0.0000	C	-5.0873	-0.4717	0.0000	H	2.0829	4.3146	0.0000
C	-1.8825	-3.2360	0.0000	C	-5.3275	-1.8962	0.0000	H	-0.3278	4.7776	0.0000
C	1.0819	-0.9429	0.0000	C	-4.3067	-2.7790	0.0000	H	-2.6798	3.9590	0.0000
C	2.1304	-1.8615	0.0000	C	-2.9317	-2.3340	0.0000	H	-4.3796	3.3619	0.0000
C	1.3452	0.4718	0.0000	C	-2.6672	-0.9338	0.0000	H	-6.7217	2.5158	0.0000
C	1.8826	3.2360	0.0000	C	3.4992	-1.3915	0.0000	H	-7.1770	0.0752	0.0000
C	0.2725	1.4002	0.0000	C	4.5840	-2.2802	0.0000	H	-6.3691	-2.2378	0.0000
C	0.5454	2.7846	0.0000	C	5.8863	-1.8076	0.0000	H	-4.4939	-3.8590	0.0000
C	-0.5458	3.7035	0.0000	C	6.1432	-0.4388	0.0000	H	4.3796	-3.3619	0.0000
C	-1.8330	3.2550	0.0000	C	3.7534	-0.0019	0.0000	H	6.7217	-2.5157	0.0000
C	-1.0819	0.9429	0.0000	C	5.0873	0.4717	0.0000	H	7.1770	-0.0752	0.0000
C	-2.1304	1.8615	0.0000	C	5.3275	1.8962	0.0000	H	6.3691	2.2377	0.0000
C	-1.3452	-0.4718	0.0000	C	4.3067	2.7790	0.0000	H	4.4939	3.8591	0.0000
C	-3.4992	1.3915	0.0000	C	2.9317	2.3340	0.0000				
C	-4.5840	2.2802	0.0000	C	2.6672	0.9338	0.0000				

Table 3.636: Table of thermodynamic data as a function of temperature for Dinaphtho[8,1,2-*abc*:8',1',2'-*jkl*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.505	502.450	502.450	∞
100	121.476	360.269	884.145	-52.388	529.483	577.464	-301.630
200	262.796	485.683	653.111	-33.486	515.097	631.210	-164.852
250	342.629	552.860	626.296	-18.359	508.399	661.010	-138.108
298.15	419.677	619.819	619.819	0.000	502.450	690.959	-121.051
300	422.594	622.424	619.827	0.779	502.229	692.126	-120.507
350	499.233	693.382	625.256	23.844	496.746	724.222	-108.082
400	570.305	764.755	638.233	50.609	491.983	757.039	-98.857
450	634.744	835.715	656.240	80.764	487.842	790.426	-91.748
500	692.376	905.634	677.694	113.970	484.224	824.271	-86.109
600	788.918	1040.756	727.042	188.229	478.243	892.871	-77.730
700	864.898	1168.304	781.063	271.068	473.750	962.359	-71.811
800	925.357	1287.890	837.025	360.692	470.594	1032.378	-67.406
900	974.171	1399.799	893.407	455.753	468.603	1102.711	-63.998
1000	1014.122	1504.574	949.342	555.232	467.622	1173.228	-61.282
1100	1047.194	1602.829	1004.331	658.348	467.443	1243.817	-59.063
1200	1074.837	1695.167	1058.092	764.490	467.924	1314.367	-57.212
1300	1098.132	1782.146	1110.476	873.171	468.873	1384.871	-55.644
1400	1117.907	1864.270	1161.413	984.000	470.150	1455.294	-54.297
1500	1134.804	1941.988	1210.884	1096.657	471.679	1525.620	-53.126
1600	1149.331	2015.702	1258.901	1210.882	473.316	1595.827	-52.097
1700	1161.891	2085.766	1305.497	1326.458	474.988	1665.902	-51.186
1800	1172.808	2152.494	1350.713	1443.205	476.611	1735.959	-50.375
1900	1182.346	2216.166	1394.601	1560.973	478.160	1805.861	-49.646
2000	1190.718	2277.030	1437.212	1679.635	479.578	1875.718	-48.988
2100	1198.101	2335.307	1478.601	1799.084	480.774	1945.492	-48.390
2200	1204.638	2391.197	1518.821	1919.227	481.754	2015.213	-47.846
2300	1210.450	2444.876	1557.925	2039.987	482.518	2084.900	-47.349
2400	1215.638	2496.504	1595.964	2161.297	482.979	2154.493	-46.890
2500	1220.284	2546.225	1632.986	2283.097	483.159	2224.218	-46.472
2600	1224.461	2594.168	1669.038	2405.338	483.016	2293.792	-46.082
2700	1228.228	2640.451	1704.164	2527.976	482.558	2363.477	-45.723
2800	1231.635	2685.182	1738.406	2650.972	481.754	2433.204	-45.391
2900	1234.726	2728.456	1771.804	2774.292	480.570	2502.903	-45.081
3000	1237.538	2770.363	1804.394	2897.907	479.066	2572.684	-44.793
3100	1240.103	2810.984	1836.213	3021.791	477.142	2642.416	-44.523
3200	1242.449	2850.394	1867.293	3145.921	474.855	2712.315	-44.273
3300	1244.599	2888.659	1897.667	3270.275	472.185	2782.346	-44.040
3400	1246.574	2925.844	1927.363	3394.835	469.093	2852.343	-43.820
3500	1248.393	2962.006	1956.410	3519.584	465.591	2922.417	-43.614
3600	1250.072	2997.198	1984.834	3644.509	461.707	2992.716	-43.422
3700	1251.623	3031.470	2012.661	3769.594	457.401	3063.141	-43.243
3800	1253.060	3064.868	2039.913	3894.830	452.644	3133.620	-43.074
3900	1254.393	3097.434	2066.613	4020.203	447.485	3204.153	-42.914
4000	1255.633	3129.208	2092.782	4145.705	441.907	3275.009	-42.766
4100	1256.787	3160.228	2118.441	4271.327	435.865	3345.915	-42.627
4200	1257.863	3190.526	2143.607	4397.060	429.394	3416.962	-42.495
4300	1258.868	3220.136	2168.300	4522.897	422.479	3488.051	-42.371
4400	1259.808	3249.088	2192.535	4648.831	415.129	3559.423	-42.255
4500	1260.688	3277.409	2216.330	4774.856	407.367	3631.035	-42.147
4600	1261.514	3305.127	2239.699	4900.967	399.121	3702.846	-42.046
4700	1262.289	3332.266	2262.658	5027.157	390.416	3774.689	-41.950
4800	1263.018	3358.849	2285.219	5153.423	381.305	3846.862	-41.862
4900	1263.704	3384.899	2307.397	5279.760	371.698	3919.050	-41.777
5000	1264.351	3410.435	2329.203	5406.163	361.713	3991.676	-41.700

3.637. Benzo[*qrs*]naphtho[3,2,1,8,7-*defgh*]pyranthrene



Formula: C₃₆H₁₆
Mass: 448.512 g/mol
CAS Number: 128345-79-9
Point Group: C_s

Length: 17.97 Å
Width: 11.69 Å
Breadth: 3.888 Å
L/B Ratio: 1.537

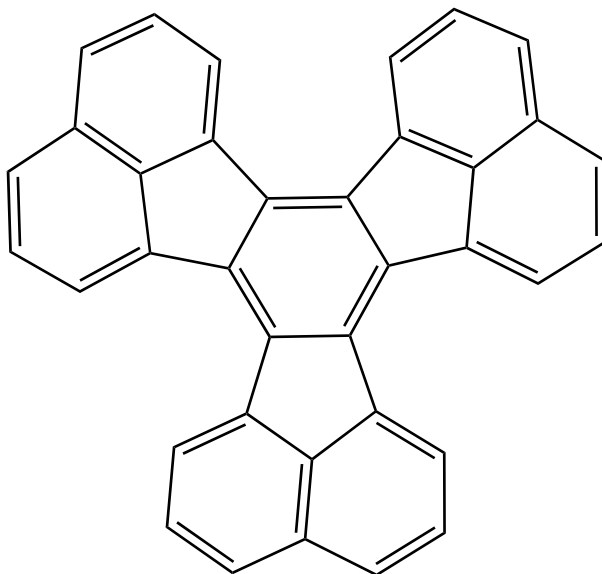
Cartesian coordinates:

C	6.3233	-0.9621	0.0000	C	3.1187	-2.8173	0.0000	H	7.0407	-1.7906	0.0000
C	6.7865	0.3582	0.0000	C	4.4467	-2.5750	0.0000	H	7.8653	0.5474	0.0000
C	5.9019	1.4172	0.0000	C	4.9592	-1.2253	0.0000	H	6.2724	2.4486	0.0000
C	4.5110	1.1848	0.0000	C	4.0357	-0.1470	0.0000	H	3.9657	3.2906	0.0000
C	3.5808	2.2633	0.0000	C	-4.7511	0.7939	0.0000	H	1.6633	4.1361	0.0000
C	2.2265	2.0261	0.0000	C	-6.1203	0.5397	0.0000	H	-0.6402	4.9849	0.0000
C	1.2739	3.1103	0.0000	C	-6.5936	-0.7747	0.0000	H	-3.0759	4.5557	0.0000
C	-0.0660	2.8756	0.0000	C	-5.7185	-1.8444	0.0000	H	-4.9528	2.9667	0.0000
C	-1.0325	3.9611	0.0000	C	-3.8419	-0.2969	0.0000	H	2.7259	-3.8460	0.0000
C	-2.3571	3.7278	0.0000	C	-4.3278	-1.6249	0.0000	H	5.1708	-3.3979	0.0000
C	-2.8934	2.3773	0.0000	C	-3.4011	-2.7099	0.0000	H	-6.8306	1.3742	0.0000
C	-4.2346	2.1374	0.0000	C	-2.4375	-0.0559	0.0000	H	-7.6740	-0.9550	0.0000
C	-1.9493	1.2810	0.0000	C	-1.5395	-1.1377	0.0000	H	-6.1000	-2.8717	0.0000
C	-0.5784	1.5203	0.0000	C	-2.0478	-2.4809	0.0000	H	-3.7923	-3.7347	0.0000
C	0.3375	0.4314	0.0000	C	-1.0916	-3.5676	0.0000	H	-1.4833	-4.5914	0.0000
C	1.7329	0.6768	0.0000	C	0.2362	-3.3332	0.0000	H	0.9620	-4.1614	0.0000
C	2.6321	-0.4035	0.0000	C	0.7762	-1.9915	0.0000				
C	2.1499	-1.7465	0.0000	C	-0.1407	-0.9000	0.0000				

Table 3.637: Table of thermodynamic data as a function of temperature for Benzo[*qrs*]naphtho[3,2,1,8,7-*defgh*]pyranthrene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-59.978	556.959	556.959	∞
100	122.115	366.786	895.236	-52.845	583.534	630.865	-329.523
200	265.262	493.224	662.147	-33.785	569.307	683.912	-178.616
250	345.735	561.025	635.095	-18.518	562.750	713.320	-149.037
298.15	423.116	628.563	628.563	0.000	556.959	742.861	-130.143
300	426.041	631.190	628.571	0.785	556.745	744.012	-129.541
350	502.777	702.689	634.043	24.026	551.438	775.656	-115.758
400	573.783	774.533	647.115	50.967	546.850	807.996	-105.511
450	638.067	845.894	665.245	81.292	542.879	840.883	-97.605
500	695.499	916.152	686.834	114.659	539.423	874.210	-91.326
600	791.617	1051.807	736.458	189.209	533.733	941.731	-81.983
700	867.213	1179.741	790.742	272.299	529.490	1010.093	-75.373
800	927.350	1299.615	846.942	362.138	526.549	1078.954	-70.447
900	975.901	1411.742	903.538	457.384	524.744	1148.103	-66.633
1000	1015.634	1516.688	959.663	557.025	523.925	1217.417	-63.590
1100	1048.527	1615.079	1014.821	660.284	523.887	1286.787	-61.103
1200	1076.018	1707.526	1068.734	766.551	524.494	1356.106	-59.029
1300	1099.186	1794.594	1121.253	875.343	525.555	1425.371	-57.271
1400	1118.852	1876.792	1172.312	986.271	526.931	1494.544	-55.761
1500	1135.655	1954.572	1221.893	1099.018	528.550	1563.615	-54.449
1600	1150.101	2028.338	1270.011	1213.324	530.267	1632.561	-53.297
1700	1162.590	2098.447	1316.698	1328.973	532.013	1701.370	-52.276
1800	1173.446	2165.213	1361.997	1445.788	533.703	1770.158	-51.368
1900	1182.929	2228.917	1405.961	1563.617	535.312	1838.785	-50.551
2000	1191.253	2289.810	1448.643	1682.335	536.786	1907.366	-49.814
2100	1198.593	2348.113	1490.096	1801.835	538.034	1975.861	-49.146
2200	1205.092	2404.024	1530.376	1922.025	539.061	2044.300	-48.537
2300	1210.871	2457.723	1569.536	2042.829	539.869	2112.703	-47.980
2400	1216.028	2509.368	1607.627	2164.179	540.370	2181.010	-47.467
2500	1220.648	2559.104	1644.697	2286.017	540.588	2249.448	-46.999
2600	1224.800	2607.061	1680.795	2408.293	540.480	2317.734	-46.563
2700	1228.544	2653.357	1715.963	2530.963	540.055	2386.129	-46.161
2800	1231.931	2698.098	1750.245	2653.990	539.281	2454.565	-45.790
2900	1235.004	2741.383	1783.680	2777.339	538.126	2522.971	-45.443
3000	1237.799	2783.299	1816.305	2900.981	536.649	2591.459	-45.120
3100	1240.349	2823.929	1848.157	3024.891	534.750	2659.897	-44.818
3200	1242.681	2863.345	1879.269	3149.044	532.487	2728.502	-44.537
3300	1244.818	2901.618	1909.672	3273.420	529.840	2797.237	-44.276
3400	1246.782	2938.809	1939.397	3398.002	526.769	2865.938	-44.029
3500	1248.589	2974.977	1968.470	3522.772	523.287	2934.715	-43.797
3600	1250.258	3010.174	1996.920	3647.715	519.422	3003.717	-43.582
3700	1251.800	3044.451	2024.771	3772.819	515.134	3072.843	-43.380
3800	1253.228	3077.854	2052.046	3898.071	510.395	3142.025	-43.189
3900	1254.553	3110.424	2078.768	4023.461	505.252	3211.258	-43.009
4000	1255.785	3142.203	2104.958	4148.979	499.690	3280.816	-42.842
4100	1256.932	3173.225	2130.636	4274.615	493.663	3350.422	-42.684
4200	1258.001	3203.527	2155.822	4400.362	487.206	3420.169	-42.535
4300	1259.000	3233.141	2180.533	4526.213	480.305	3489.958	-42.394
4400	1259.935	3262.095	2204.786	4652.160	472.968	3560.028	-42.262
4500	1260.810	3290.420	2228.598	4778.198	465.217	3630.340	-42.139
4600	1261.630	3318.140	2251.983	4904.320	456.984	3700.849	-42.024
4700	1262.401	3345.281	2274.957	5030.522	448.290	3771.392	-41.913
4800	1263.125	3371.867	2297.533	5156.799	439.190	3842.263	-41.811
4900	1263.807	3397.918	2319.725	5283.146	429.593	3913.149	-41.714
5000	1264.450	3423.457	2341.545	5409.559	419.619	3984.472	-41.625

3.638. Decacyclene



Other names: Benzo[1,2-*a*,3,4-*a'*,5,6-*a''*]triacenaphthylene
Trinaphthylenebenzene

Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 191-48-0
Point Group: D₃

Length: 14.99 Å
Width: 14.41 Å
Breadth: 4.969 Å
L/B Ratio: 1.040

Cartesian coordinates:

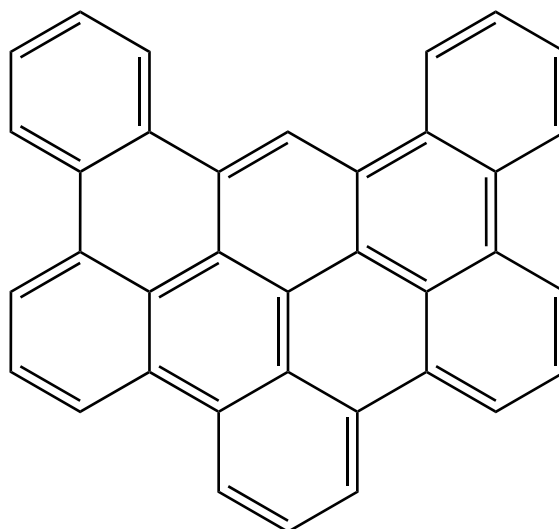
C	1.3308	0.4764	-0.0600	C	-0.8288	-2.7454	-0.1168	C	1.1275	3.8188	-0.6288
C	1.0509	-0.9530	0.0161	C	-2.6310	-4.9229	-0.2941	C	0.6825	5.1685	-0.6660
C	-0.2464	-1.3970	-0.0157	C	-1.2735	-5.0964	-0.3932	C	-0.6020	5.5340	-0.3497
C	-1.3434	-0.4390	0.0616	C	-0.3556	-4.0134	-0.3238	C	-1.5529	4.5356	-0.0023
C	-1.0739	0.9047	0.0954	C	-2.2457	-2.5725	-0.0450	H	6.6667	0.0451	0.1434
C	0.2944	1.3732	-0.0936	C	-2.6076	-1.1932	0.0492	H	5.7289	2.3360	0.0059
C	2.7920	0.6550	-0.0470	C	-3.9419	-0.8862	0.0404	H	3.3113	2.7548	-0.0492
C	5.5844	0.2059	0.0975	C	-4.8975	-1.9368	-0.0155	H	2.0266	-3.7748	0.4583
C	5.0573	1.4704	0.0200	C	-4.5393	-3.2589	-0.0958	H	4.4247	-4.2933	0.5315
C	3.6583	1.7152	-0.0357	C	-3.1631	-3.6139	-0.1350	H	6.1598	-2.5321	0.3467
C	3.3512	-0.6570	0.0449	C	-1.9347	2.0880	0.2593	H	-3.3167	-5.7748	-0.3503
C	2.3374	-1.6618	0.1158	C	-2.9160	4.7421	0.3461	H	-0.8663	-6.1035	-0.5362
C	2.7404	-2.9541	0.3215	C	-3.7064	3.6665	0.6654	H	0.7113	-4.2248	-0.4605
C	4.1294	-3.2477	0.3900	C	-3.2306	2.3273	0.6302	H	-4.3047	0.1480	0.0563
C	5.0959	-2.2787	0.2918	C	-1.1027	3.2200	-0.0021	H	-5.9587	-1.6643	-0.0003
C	4.7144	-0.9180	0.1346	C	0.2492	2.8354	-0.2604	H	-5.2962	-4.0490	-0.1429

H	-3.3138	5.7622	0.3641	H	-3.9149	1.5204	0.9181	H	1.4075	5.9378	-0.9543
H	-4.7501	3.8305	0.9559	H	2.1638	3.6007	-0.9130	H	-0.9126	6.5840	-0.3678

Table 3.638: Table of thermodynamic data as a function of temperature for Decaylene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K_f
	C_p°	S°	$-\frac{G^\circ - H^\circ(298\text{ K})}{T}$	$H^\circ(T) - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.0	0.0	∞	-64.199	742.150	742.150	∞
100	140.498	380.666	939.707	-55.904	771.134	827.148	-432.049
200	279.504	518.450	694.619	-35.234	755.822	889.264	-232.247
250	360.315	589.432	666.447	-19.254	748.582	923.460	-192.942
298.15	439.231	659.659	659.659	0.000	742.150	957.742	-167.789
300	442.228	662.385	659.668	0.815	741.912	959.077	-166.987
350	521.023	736.533	665.344	24.916	736.016	995.752	-148.605
400	594.078	810.948	678.895	52.821	730.936	1033.201	-134.919
450	660.214	884.809	697.679	84.208	726.566	1071.253	-124.345
500	719.266	957.486	720.038	118.724	722.796	1109.785	-115.936
600	818.042	1097.719	771.404	195.789	716.692	1187.789	-103.404
700	895.792	1229.893	827.561	281.632	712.265	1266.685	-94.519
800	957.802	1353.707	885.677	374.425	709.324	1346.093	-87.889
900	1008.049	1469.521	944.186	472.802	707.675	1425.780	-82.748
1000	1049.341	1577.936	1002.199	575.737	707.146	1505.607	-78.643
1100	1083.666	1679.607	1059.209	682.438	707.513	1585.455	-75.285
1200	1112.465	1775.169	1114.931	792.286	708.623	1665.211	-72.483
1300	1136.820	1865.202	1169.215	904.784	710.267	1744.867	-70.108
1400	1157.557	1950.229	1221.993	1019.530	712.297	1824.385	-68.067
1500	1175.324	2030.713	1273.249	1136.196	714.628	1903.751	-66.293
1600	1190.634	2107.068	1322.997	1254.513	717.105	1982.943	-64.735
1700	1203.899	2179.657	1371.272	1374.255	719.650	2061.948	-63.355
1800	1215.449	2248.804	1418.118	1495.235	722.172	2140.885	-62.126
1900	1225.554	2314.797	1463.588	1617.297	724.641	2219.615	-61.020
2000	1234.437	2377.890	1507.737	1740.305	726.996	2298.252	-60.023
2100	1242.279	2438.312	1550.622	1864.149	729.142	2376.757	-59.117
2200	1249.231	2496.267	1592.298	1988.732	731.081	2455.167	-58.292
2300	1255.417	2551.936	1632.819	2113.970	732.813	2533.496	-57.536
2400	1260.943	2605.485	1672.238	2239.793	734.247	2611.689	-56.841
2500	1265.896	2657.062	1710.606	2366.139	735.403	2689.976	-56.203
2600	1270.352	2706.799	1747.970	2492.956	736.237	2768.071	-55.610
2700	1274.372	2754.820	1784.377	2620.195	736.757	2846.238	-55.063
2800	1278.011	2801.232	1819.869	2747.817	736.930	2924.415	-54.555
2900	1281.313	2846.138	1854.488	2875.786	736.721	3002.526	-54.080
3000	1284.319	2889.628	1888.271	3004.070	736.188	3080.685	-53.638
3100	1287.062	2931.786	1921.256	3132.641	735.231	3158.765	-53.224
3200	1289.571	2972.689	1953.478	3261.475	733.906	3236.980	-52.837
3300	1291.871	3012.407	1984.968	3390.548	732.192	3315.295	-52.476
3400	1293.986	3051.005	2015.757	3519.843	730.050	3393.551	-52.134
3500	1295.933	3088.543	2045.874	3649.340	727.491	3471.853	-51.813
3600	1297.730	3125.076	2075.347	3779.024	724.542	3550.353	-51.513
3700	1299.392	3160.655	2104.201	3908.882	721.163	3628.956	-51.231
3800	1300.932	3195.328	2132.460	4038.899	717.323	3707.584	-50.963
3900	1302.361	3229.139	2160.148	4169.064	713.074	3786.245	-50.710
4000	1303.689	3262.129	2187.287	4299.368	708.395	3865.206	-50.473
4100	1304.926	3294.336	2213.897	4429.799	703.242	3944.193	-50.249
4200	1306.080	3325.796	2239.998	4560.350	697.650	4023.300	-50.036
4300	1307.158	3356.541	2265.608	4691.013	691.602	4102.426	-49.834
4400	1308.166	3386.604	2290.745	4821.779	685.110	4181.818	-49.643
4500	1309.110	3416.013	2315.425	4952.644	678.193	4261.433	-49.464
4600	1309.996	3444.795	2339.665	5083.599	670.783	4341.223	-49.295
4700	1310.828	3472.977	2363.479	5214.641	662.901	4421.029	-49.133
4800	1311.610	3500.583	2386.882	5345.763	654.604	4501.147	-48.981
4900	1312.346	3527.635	2409.888	5476.961	645.798	4581.262	-48.836
5000	1313.040	3554.155	2432.509	5608.231	636.605	4661.804	-48.701

3.639. Dibenzo[*fg,ij*]phenanthro[9,10,1,2,3-*pqrst*]pentaphene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 188-00-1
Point Group: C_{2v}

Length: 15.91 Å
Width: 14.11 Å
Breadth: 3.890 Å
L/B Ratio: 1.128

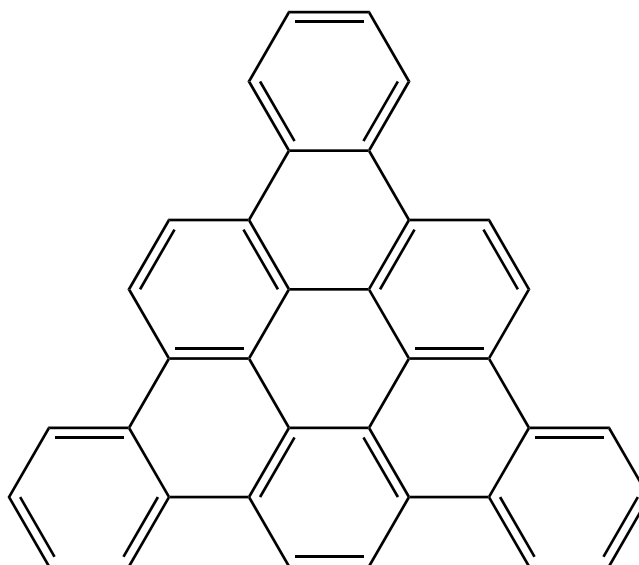
Cartesian coordinates:

C	1.2147	2.8687	0.0000	C	2.5016	-3.5329	0.0000	H	2.1485	4.8163	0.0000
C	1.1946	4.2671	0.0000	C	3.6968	-4.2249	0.0000	H	-0.0103	6.0529	0.0000
C	-0.0084	4.9580	0.0000	C	4.9071	-3.5259	0.0000	H	-2.1647	4.8091	0.0000
C	-1.2090	4.2630	0.0000	C	4.9050	-2.1448	0.0000	H	0.0054	-3.1869	0.0000
C	-0.0037	2.1563	0.0000	C	-2.4841	2.1349	0.0000	H	5.8514	0.1937	0.0000
C	-1.2244	2.8646	0.0000	C	-3.7060	2.8152	0.0000	H	5.8456	2.6818	0.0000
C	-0.0012	0.7127	0.0000	C	-4.9049	2.1171	0.0000	H	3.6927	3.9286	0.0000
C	0.0036	-2.0801	0.0000	C	-4.9020	0.7297	0.0000	H	1.5448	-4.0774	0.0000
C	1.2230	0.0115	0.0000	C	-2.4751	0.7239	0.0000	H	3.6991	-5.3197	0.0000
C	1.2203	-1.3988	0.0000	C	-3.6981	0.0186	0.0000	H	5.8542	-4.0751	0.0000
C	2.4768	2.1434	0.0000	C	-1.2155	-1.4030	0.0000	H	5.8542	-1.5874	0.0000
C	2.4727	0.7323	0.0000	C	-1.2230	0.0073	0.0000	H	-3.7062	3.9159	0.0000
C	3.6980	0.0312	0.0000	C	-2.4737	-2.1352	0.0000	H	-5.8547	2.6618	0.0000
C	4.8995	0.7464	0.0000	C	-3.6925	-1.4371	0.0000	H	-5.8520	0.1737	0.0000
C	4.8976	2.1339	0.0000	C	-4.8977	-2.1615	0.0000	H	-5.8488	-1.6072	0.0000
C	3.6964	2.8278	0.0000	C	-4.8952	-3.5425	0.0000	H	-5.8404	-4.0949	0.0000
C	3.6974	-1.4245	0.0000	C	-3.6824	-4.2375	0.0000	H	-3.6811	-5.3323	0.0000
C	2.4810	-2.1268	0.0000	C	-2.4896	-3.5414	0.0000	H	-1.5310	-4.0827	0.0000

Table 3.639: Table of thermodynamic data as a function of temperature for Dibenzof[*g,i*]phenanthro[9,10,1,2,3-*pqrst*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-63.505	544.892	544.892	∞
100	137.333	387.160	939.491	-55.233	574.547	629.912	-329.026
200	276.439	522.841	697.162	-34.864	558.934	691.498	-180.597
250	356.536	593.068	669.284	-19.054	551.524	725.493	-151.580
298.15	434.748	662.566	662.566	0.000	544.892	759.618	-133.079
300	437.722	665.265	662.575	0.807	544.646	760.948	-132.490
350	516.054	738.679	668.194	24.670	538.512	797.497	-119.017
400	588.937	812.416	681.614	52.321	533.178	834.856	-109.019
450	655.122	885.672	700.225	83.451	528.551	872.850	-101.316
500	714.363	957.823	722.389	117.717	524.531	911.352	-95.206
600	813.701	1097.209	773.344	194.319	517.964	989.367	-86.130
700	892.045	1228.759	829.105	279.758	513.133	1068.347	-79.719
800	954.584	1352.109	886.855	372.203	509.845	1147.892	-74.948
900	1005.276	1467.570	945.035	470.281	507.897	1227.758	-71.256
1000	1046.938	1575.712	1002.754	572.958	507.110	1307.794	-68.311
1100	1081.567	1677.169	1059.501	679.435	507.252	1387.875	-65.903
1200	1110.621	1772.560	1114.988	789.086	508.165	1467.884	-63.894
1300	1135.188	1862.454	1169.062	901.410	509.636	1547.808	-62.190
1400	1156.104	1947.366	1221.650	1016.002	511.512	1627.607	-60.726
1500	1174.024	2027.756	1272.735	1132.531	513.705	1707.264	-59.451
1600	1189.465	2104.030	1322.328	1250.724	516.059	1786.756	-58.330
1700	1202.842	2176.552	1370.461	1370.355	518.492	1866.068	-57.336
1800	1214.490	2245.642	1417.178	1491.235	520.914	1945.319	-56.451
1900	1224.681	2311.585	1462.530	1613.205	523.292	2024.367	-55.653
2000	1233.638	2374.636	1506.571	1736.130	525.563	2103.328	-54.932
2100	1241.546	2435.020	1549.355	1859.897	527.632	2182.161	-54.277
2200	1248.556	2492.942	1590.938	1984.409	529.501	2260.901	-53.680
2300	1254.794	2548.583	1631.373	2109.583	531.168	2339.564	-53.132
2400	1260.366	2602.106	1670.712	2235.346	532.542	2418.094	-52.627
2500	1265.361	2653.660	1709.005	2361.637	533.643	2496.720	-52.165
2600	1269.853	2703.378	1746.300	2488.401	534.425	2575.156	-51.734
2700	1273.907	2751.380	1782.641	2615.593	534.897	2653.666	-51.337
2800	1277.576	2797.776	1818.072	2743.170	535.025	2732.188	-50.969
2900	1280.906	2842.667	1852.633	2871.097	534.774	2810.645	-50.624
3000	1283.937	2886.143	1886.363	2999.341	534.201	2889.152	-50.304
3100	1286.702	2928.289	1919.297	3127.875	533.207	2967.581	-50.002
3200	1289.232	2969.181	1951.470	3256.674	531.848	3046.146	-49.722
3300	1291.552	3008.889	1982.915	3385.715	530.101	3124.813	-49.461
3400	1293.684	3047.477	2013.660	3514.978	527.928	3203.420	-49.214
3500	1295.648	3085.007	2043.737	3644.446	525.339	3282.076	-48.981
3600	1297.460	3121.532	2073.170	3774.102	522.363	3360.930	-48.765
3700	1299.136	3157.104	2101.987	3903.933	518.957	3439.888	-48.562
3800	1300.688	3191.771	2130.212	4033.925	515.093	3518.871	-48.369
3900	1302.129	3225.576	2157.866	4164.067	510.819	3597.889	-48.187
4000	1303.468	3258.560	2184.973	4294.348	506.118	3677.206	-48.018
4100	1304.715	3290.761	2211.552	4424.758	500.943	3756.550	-47.858
4200	1305.879	3322.216	2237.624	4555.288	495.330	3836.014	-47.707
4300	1306.965	3352.957	2263.206	4685.931	489.263	3915.499	-47.563
4400	1307.982	3383.015	2288.315	4816.679	482.752	3995.249	-47.429
4500	1308.934	3412.420	2312.970	4947.525	475.817	4075.223	-47.303
4600	1309.827	3441.199	2337.185	5078.464	468.390	4155.373	-47.185
4700	1310.666	3469.377	2360.975	5209.489	460.491	4235.539	-47.072
4800	1311.454	3496.980	2384.356	5340.595	452.178	4316.017	-46.967
4900	1312.197	3524.029	2407.339	5471.778	443.357	4396.493	-46.866
5000	1312.897	3550.546	2429.939	5603.033	434.149	4477.396	-46.774

3.640. Tribenzo[*fgh,pqr,za1b1*]trinaphthylene



Formula: $C_{36}H_{18}$
Mass: 450.528 g/mol
CAS Number: 97269-75-5
Point Group: D_{3h}

Length: 15.91 Å
Width: 14.11 Å
Breadth: 3.886 Å
L/B Ratio: 1.128

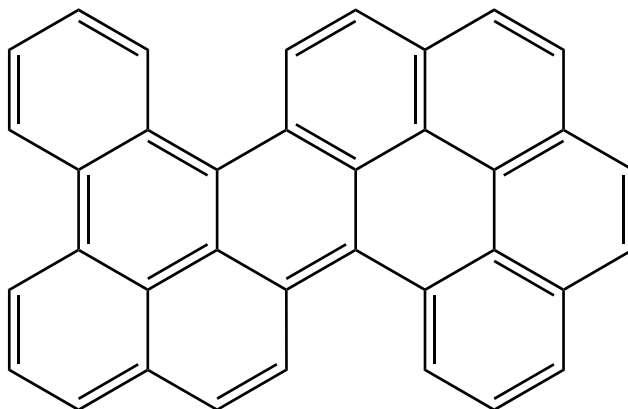
Cartesian coordinates:

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C	-1.7561	-3.2931	0.0000	C	-3.7728	-0.1195	0.0000	H	-2.5726	-4.0315	0.0000
C	-2.0825	-1.9229	0.0000	C	-5.1227	0.2835	0.0000	H	4.7778	-0.2122	0.0000
C	-1.0500	-0.9724	0.0000	C	-6.1392	-0.6480	0.0000	H	4.2376	2.2169	0.0000
C	0.3042	-1.3984	0.0000	C	-5.8353	-2.0149	0.0000	H	-2.2051	4.2438	0.0000
C	0.6066	-2.7688	0.0000	C	-4.5197	-2.4278	0.0000	H	-4.0387	2.5613	0.0000
C	1.3671	-0.4231	0.0000	C	3.0249	-2.2580	0.0000	H	-5.3527	1.3600	0.0000
C	2.7066	-0.8421	0.0000	C	1.9898	-3.2076	0.0000	H	-7.1848	-0.3235	0.0000
C	3.7300	0.1257	0.0000	C	2.3157	-4.5782	0.0000	H	-6.6448	-2.7519	0.0000
C	3.4318	1.4669	0.0000	C	3.6307	-4.9928	0.0000	H	-4.2718	-3.5003	0.0000
C	1.0590	0.9626	0.0000	C	4.6625	-4.0461	0.0000	H	1.4985	-5.3155	0.0000
C	2.0946	1.9098	0.0000	C	4.3624	-2.7004	0.0000	H	3.8725	-6.0605	0.0000
C	-0.3171	1.3955	0.0000	C	0.4430	3.7487	0.0000	H	5.7055	-4.3787	0.0000
C	-0.6240	2.7650	0.0000	C	1.7830	3.3271	0.0000	H	5.1672	-1.9495	0.0000
C	-1.9739	3.1675	0.0000	C	2.8069	4.2947	0.0000	H	3.8542	3.9557	0.0000
C	-2.9863	2.2386	0.0000	C	2.5084	5.6408	0.0000	H	3.3122	6.3841	0.0000
C	-2.7012	0.8591	0.0000	C	1.1727	6.0610	0.0000	H	0.9391	7.1306	0.0000
C	-1.3631	0.4358	0.0000	C	0.1573	5.1281	0.0000	H	-0.8954	5.4497	0.0000

Table 3.640: Table of thermodynamic data as a function of temperature for Tribenzo[*fgh,pqr,za1b1*]trinaphthylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-63.567	530.359	530.359	∞
100	137.408	379.239	931.309	-55.207	560.040	616.197	-321.862
200	276.272	514.789	689.079	-34.858	544.407	678.581	-177.223
250	356.487	584.992	661.204	-19.053	536.992	712.980	-148.966
298.15	434.743	654.487	654.487	0.000	530.359	747.493	-130.955
300	437.718	657.185	654.495	0.807	530.113	748.838	-130.382
350	516.042	730.599	660.114	24.670	523.978	785.792	-117.271
400	588.896	804.333	673.534	52.319	518.643	823.555	-107.543
450	655.049	877.582	692.145	83.447	514.014	861.953	-100.051
500	714.264	949.723	714.307	117.708	509.989	900.860	-94.110
600	813.571	1089.088	765.258	194.298	503.410	979.686	-85.287
700	891.906	1220.617	821.012	279.724	498.565	1059.479	-79.058
800	954.449	1343.948	878.755	372.155	495.263	1139.839	-74.422
900	1005.151	1459.394	936.928	470.220	493.303	1220.521	-70.836
1000	1046.824	1567.524	994.639	572.885	492.503	1301.376	-67.975
1100	1081.465	1668.971	1051.379	679.351	492.635	1382.276	-65.637
1200	1110.529	1764.353	1106.859	788.992	493.538	1463.106	-63.686
1300	1135.106	1854.240	1160.926	901.307	495.000	1543.851	-62.031
1400	1156.031	1939.146	1213.509	1015.892	496.868	1624.471	-60.609
1500	1173.958	2019.531	1264.589	1132.414	499.055	1704.951	-59.370
1600	1189.406	2095.802	1314.176	1250.601	501.403	1785.265	-58.282
1700	1202.788	2168.320	1362.305	1370.226	503.830	1865.400	-57.316
1800	1214.441	2237.407	1409.018	1491.101	506.247	1945.474	-56.455
1900	1224.637	2303.348	1454.366	1613.066	508.620	2025.346	-55.680
2000	1233.598	2366.396	1498.403	1735.987	510.887	2105.131	-54.979
2100	1241.509	2426.779	1541.183	1859.751	512.952	2184.788	-54.342
2200	1248.522	2484.699	1582.763	1984.259	514.818	2264.352	-53.761
2300	1254.762	2540.338	1623.195	2109.429	516.481	2343.839	-53.229
2400	1260.337	2593.861	1662.532	2235.189	517.852	2423.194	-52.738
2500	1265.334	2645.413	1700.822	2361.477	518.950	2502.645	-52.289
2600	1269.828	2695.130	1738.114	2488.239	519.730	2581.906	-51.870
2700	1273.884	2743.131	1774.453	2615.428	520.199	2661.241	-51.484
2800	1277.554	2789.526	1809.882	2743.003	520.325	2740.587	-51.125
2900	1280.886	2834.416	1844.441	2870.928	520.072	2819.869	-50.790
3000	1283.918	2877.892	1878.169	2999.171	519.497	2899.201	-50.479
3100	1286.684	2920.037	1911.101	3127.703	518.501	2978.455	-50.186
3200	1289.215	2960.929	1943.272	3256.500	517.140	3057.846	-49.913
3300	1291.536	3000.636	1974.715	3385.539	515.391	3137.337	-49.659
3400	1293.669	3039.224	2005.459	3514.801	513.217	3216.771	-49.419
3500	1295.634	3076.753	2035.534	3644.267	510.627	3296.251	-49.193
3600	1297.446	3113.278	2064.966	3773.922	507.649	3375.931	-48.982
3700	1299.123	3148.850	2093.782	3903.752	504.242	3455.714	-48.785
3800	1300.676	3183.516	2122.005	4033.743	500.376	3535.523	-48.598
3900	1302.117	3217.321	2149.658	4163.883	496.102	3615.366	-48.421
4000	1303.457	3250.305	2176.764	4294.163	491.399	3695.509	-48.257
4100	1304.705	3282.506	2203.342	4424.572	486.223	3775.678	-48.102
4200	1305.869	3313.960	2229.412	4555.101	480.610	3855.968	-47.955
4300	1306.956	3344.701	2254.993	4685.743	474.541	3936.279	-47.815
4400	1307.973	3374.759	2280.102	4816.490	468.029	4016.854	-47.685
4500	1308.925	3404.164	2304.756	4947.335	461.094	4097.654	-47.563
4600	1309.819	3432.942	2328.970	5078.273	453.666	4178.630	-47.449
4700	1310.658	3461.120	2352.759	5209.297	445.766	4259.621	-47.339
4800	1311.447	3488.723	2376.139	5340.403	437.452	4340.924	-47.238
4900	1312.190	3515.771	2399.121	5471.585	428.631	4422.226	-47.141
5000	1312.890	3542.288	2421.721	5602.839	419.422	4503.955	-47.052

3.641. Dibenzo[*j,lm*]phenanthro[5,4,3-*abcd*]perylene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 117726-80-4
Point Group: C₁

Length: 15.51 Å
Width: 11.33 Å
Breadth: 5.978 Å
L/B Ratio: 1.369

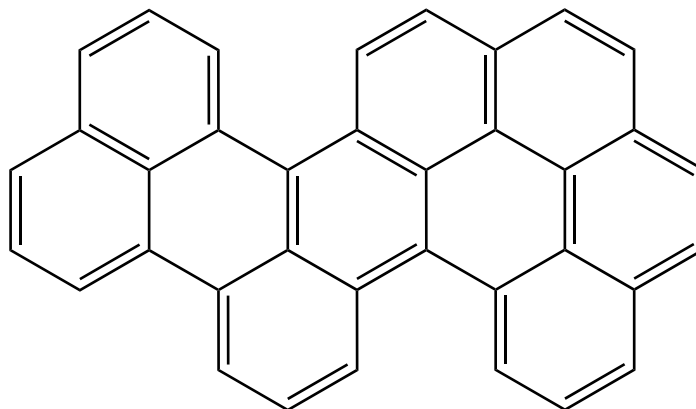
Cartesian coordinates:

C	2.0877	-1.4695	-0.4037	C	-0.2812	1.4148	0.1548	H	1.1560	-3.2611	-1.1752
C	2.1017	-2.7454	-0.9588	C	-0.3918	-1.3920	0.1357	H	3.2669	-4.4152	-1.6687
C	3.3006	-3.4084	-1.2390	C	-1.6907	-3.3946	0.6724	H	5.4531	-3.3402	-1.1623
C	4.5132	-2.8104	-0.9707	C	-0.5028	-2.7973	0.4378	H	6.7193	-1.4062	-0.3729
C	3.3358	-0.8143	-0.2222	C	-2.9153	-2.6475	0.5943	H	6.7839	0.9571	0.3918
C	4.5447	-1.4975	-0.4669	C	-5.2778	-1.1807	0.4400	H	5.6225	3.0494	0.8923
C	5.7947	-0.8383	-0.2173	C	-5.3196	-2.5323	0.7677	H	3.5132	4.3476	1.0949
C	5.8307	0.4526	0.1967	C	-4.1482	-3.2676	0.8364	H	1.0772	4.4661	0.9893
C	3.3841	0.5628	0.1670	C	-1.5842	-0.6185	0.1080	H	-1.0969	3.3984	0.5622
C	4.6181	1.1965	0.3714	C	-1.5330	0.7816	-0.0500	H	-1.7466	-4.4581	0.9322
C	4.6527	2.5686	0.7208	C	-4.0626	-0.5428	0.1874	H	0.4217	-3.3881	0.5015
C	3.4900	3.2838	0.8319	C	-2.8572	-1.2728	0.2840	H	-6.2109	-0.6017	0.3642
C	2.1736	1.2992	0.2883	C	-4.0084	0.8479	-0.2289	H	-6.2831	-3.0136	0.9649
C	2.2371	2.6619	0.6075	C	-2.7644	1.4879	-0.3879	H	-4.1779	-4.3348	1.0834
C	1.0209	3.4067	0.7139	C	-2.7570	2.7775	-0.9523	H	-1.7984	3.2800	-1.1412
C	-0.1728	2.8092	0.4817	C	-3.9297	3.4336	-1.2734	H	-3.8939	4.4366	-1.7111
C	0.8523	-0.7624	-0.0676	C	-5.1621	2.8195	-1.0412	H	-6.0921	3.3470	-1.2757
C	0.9056	0.6438	0.1067	C	-5.1956	1.5368	-0.5321	H	-6.1581	1.0284	-0.3669

Table 3.641: Table of thermodynamic data as a function of temperature for Dibenzo[*j,lm*]phenanthro[5,4,3-*abcd*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-62.706	585.844	585.844	∞
100	131.661	376.804	926.833	-55.003	615.729	672.130	-351.077
200	275.729	510.079	684.838	-34.952	599.798	734.914	-191.936
250	357.564	580.348	656.870	-19.130	592.399	769.548	-160.785
298.15	436.800	650.123	650.123	0.000	585.844	804.279	-140.903
300	439.802	652.835	650.132	0.811	585.601	805.632	-140.270
350	518.693	726.617	655.779	24.793	579.587	842.794	-125.778
400	591.818	800.725	669.266	52.583	574.392	880.747	-115.011
450	658.059	874.325	687.970	83.860	569.911	919.316	-106.709
500	717.254	946.783	710.240	118.271	566.037	958.378	-100.119
600	816.370	1086.678	761.425	195.152	559.749	1037.470	-90.318
700	894.459	1218.620	817.413	280.845	555.172	1117.483	-83.386
800	956.764	1342.276	875.377	373.519	552.113	1198.026	-78.221
900	1007.253	1457.983	933.754	471.805	550.373	1278.862	-74.222
1000	1048.735	1566.323	991.653	574.671	549.774	1359.847	-71.030
1100	1083.206	1667.944	1048.563	681.319	550.088	1440.859	-68.419
1200	1112.118	1763.471	1104.199	791.127	551.157	1521.783	-66.240
1300	1136.558	1853.480	1158.408	903.594	552.772	1602.610	-64.392
1400	1157.360	1938.490	1211.120	1018.317	554.779	1683.301	-62.803
1500	1175.177	2018.962	1262.318	1134.967	557.092	1763.842	-61.421
1600	1190.526	2095.309	1312.014	1253.271	559.557	1844.209	-60.206
1700	1203.819	2167.892	1360.243	1373.004	562.092	1924.390	-59.128
1800	1215.391	2237.036	1407.048	1493.977	564.608	2004.504	-58.168
1900	1225.514	2303.026	1452.482	1616.033	567.072	2084.411	-57.303
2000	1234.410	2366.117	1496.598	1739.039	569.424	2164.225	-56.523
2100	1242.263	2426.538	1539.452	1862.881	571.567	2243.908	-55.813
2200	1249.222	2484.492	1581.100	1987.462	573.505	2323.495	-55.166
2300	1255.414	2540.161	1621.596	2112.700	575.236	2403.001	-54.573
2400	1260.945	2593.710	1660.993	2238.523	576.670	2482.372	-54.026
2500	1265.902	2645.287	1699.339	2364.870	577.827	2561.837	-53.526
2600	1270.360	2695.025	1736.684	2491.687	578.662	2641.109	-53.059
2700	1274.383	2743.046	1773.073	2618.927	579.183	2720.454	-52.629
2800	1278.023	2789.459	1808.548	2746.550	579.357	2799.808	-52.230
2900	1281.327	2834.365	1843.151	2874.520	579.149	2879.096	-51.857
3000	1284.333	2877.855	1876.920	3002.806	578.617	2958.433	-51.510
3100	1287.077	2920.014	1909.892	3131.378	577.662	3037.690	-51.184
3200	1289.586	2960.917	1942.100	3260.213	576.339	3117.082	-50.880
3300	1291.887	3000.635	1973.578	3389.289	574.626	3196.574	-50.597
3400	1294.001	3039.234	2004.356	3518.584	572.486	3276.007	-50.329
3500	1295.949	3076.772	2034.463	3648.083	569.928	3355.486	-50.077
3600	1297.746	3113.306	2063.925	3777.769	566.981	3435.163	-49.842
3700	1299.408	3148.886	2092.770	3907.628	563.604	3514.943	-49.621
3800	1300.947	3183.559	2121.021	4037.647	559.765	3594.748	-49.412
3900	1302.376	3217.371	2148.700	4167.814	555.517	3674.586	-49.215
4000	1303.704	3250.361	2175.831	4298.118	550.840	3754.724	-49.031
4100	1304.940	3282.568	2202.434	4428.551	545.688	3834.888	-48.856
4200	1306.094	3314.028	2228.527	4559.104	540.097	3915.171	-48.691
4300	1307.171	3344.774	2254.130	4689.768	534.051	3995.475	-48.534
4400	1308.179	3374.837	2279.260	4820.536	527.560	4076.043	-48.388
4500	1309.123	3404.246	2303.935	4951.401	520.645	4156.834	-48.250
4600	1310.008	3433.029	2328.168	5082.358	513.236	4237.802	-48.121
4700	1310.840	3461.211	2351.977	5213.401	505.355	4318.784	-47.997
4800	1311.622	3488.817	2375.374	5344.525	497.059	4400.078	-47.882
4900	1312.358	3515.869	2398.375	5475.724	488.255	4481.370	-47.771
5000	1313.052	3542.390	2420.991	5606.995	479.062	4563.089	-47.669

3.642. Tribenzo[*jk,qr,uv*]naphtho[2,1,8,7-*defg*]pentacene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 117726-82-6
Point Group: C₁

Length: 16.64 Å
Width: 11.33 Å
Breadth: 5.823 Å
L/B Ratio: 1.469

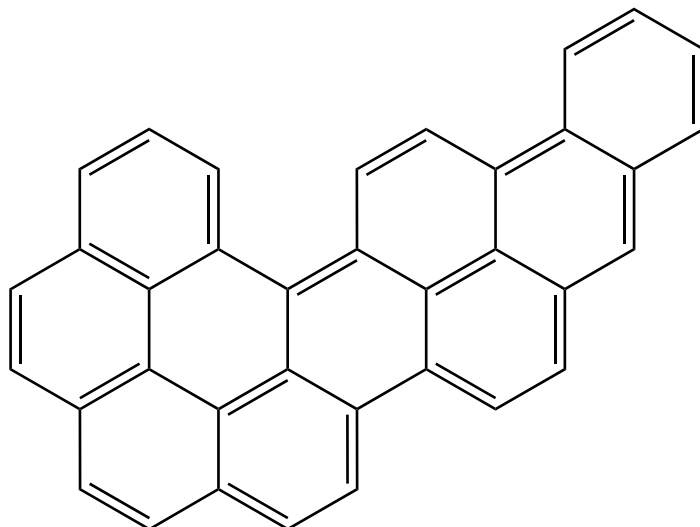
Cartesian coordinates:

C	-5.0652	-1.7281	-0.6349	C	2.0909	2.7133	-0.5009	H	0.7610	4.4167	-0.7955
C	-3.9002	-1.0543	-0.3272	C	0.8035	3.3436	-0.5763	H	-1.3017	3.1278	-0.4372
C	-3.9652	0.2925	0.1301	C	-0.3251	2.6265	-0.3840	H	5.4209	3.4413	-0.7404
C	-5.2293	0.8769	0.3594	C	4.6019	1.4790	-0.3140	H	3.1958	4.5360	-0.8936
C	-6.4080	0.1596	0.0258	C	4.5037	2.8584	-0.5984	H	6.9420	-0.9415	0.3314
C	-6.3213	-1.1109	-0.4782	C	3.2734	3.4629	-0.6837	H	6.7813	1.4479	-0.3307
C	-2.7755	1.0411	0.3901	C	4.7856	-1.2452	0.4104	H	1.5801	-3.3506	1.0334
C	-1.4783	0.4587	0.0397	C	5.9678	-0.4579	0.1948	H	3.7907	-4.3141	1.4934
C	-1.4059	-0.9473	-0.1706	C	5.8808	0.8460	-0.1631	H	5.8643	-3.0177	1.0378
C	-2.5966	-1.7079	-0.4051	C	2.4725	-2.7395	0.8399	H	-3.4333	-3.6201	-0.9147
C	-0.3065	1.2056	-0.1378	C	3.7267	-3.2937	1.1007	H	-1.2201	-4.7431	-1.0836
C	0.9605	0.5453	-0.1199	C	4.8791	-2.5715	0.8619	H	0.8530	-3.4908	-0.6393
C	1.0441	-0.8487	0.0115	C	-2.5142	-3.0472	-0.7171	H	-2.0046	2.8457	1.2812
C	-0.1483	-1.6019	-0.2142	C	-1.2634	-3.6847	-0.8063	H	-4.2103	3.8076	1.7801
C	2.1593	1.3366	-0.2501	C	-0.1176	-2.9824	-0.5575	H	-6.2944	2.6119	1.1253
C	3.4323	0.7184	-0.1480	C	-5.3091	2.1680	0.9441	H	-7.3818	0.6375	0.1814
C	3.5163	-0.6715	0.1849	C	-4.1625	2.8285	1.2917	H	-7.2252	-1.6669	-0.7479
C	2.3365	-1.4486	0.3320	C	-2.8995	2.2680	1.0123	H	-5.0118	-2.7685	-0.9907

Table 3.642: Table of thermodynamic data as a function of temperature for Tribenzo[*jk,qr,uv*]naphtho[2,1,8,7-*defg*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-62.598	612.828	612.828	∞
100	131.095	376.085	925.489	-54.940	642.776	699.249	-365.243
200	275.434	509.059	683.714	-34.931	626.803	762.123	-199.042
250	357.359	579.272	655.761	-19.122	619.392	796.810	-166.481
298.15	436.660	649.017	649.017	0.000	612.828	831.594	-145.689
300	439.665	651.728	649.026	0.811	612.586	832.949	-145.026
350	518.607	725.492	654.671	24.788	606.566	870.166	-129.863
400	591.771	799.592	668.156	52.574	601.368	908.176	-118.593
450	658.040	873.188	686.857	83.849	596.885	946.802	-109.900
500	717.255	945.645	709.124	118.260	593.011	985.921	-102.996
600	816.396	1085.543	760.306	195.142	586.724	1065.127	-92.726
700	894.496	1217.490	816.292	280.839	582.150	1145.253	-85.458
800	956.804	1341.151	874.256	373.517	579.095	1225.908	-80.042
900	1007.293	1456.862	932.632	471.807	577.359	1306.857	-75.846
1000	1048.774	1565.207	990.531	574.676	576.764	1387.953	-72.498
1100	1083.243	1666.832	1047.442	681.328	577.082	1469.076	-69.759
1200	1112.152	1762.362	1103.079	791.140	578.155	1550.112	-67.473
1300	1136.589	1852.373	1157.289	903.610	579.772	1631.050	-65.535
1400	1157.389	1937.385	1210.002	1018.336	581.783	1711.851	-63.869
1500	1175.204	2017.860	1261.201	1134.989	584.099	1792.502	-62.419
1600	1190.550	2094.207	1310.898	1253.295	586.566	1872.980	-61.145
1700	1203.841	2166.792	1359.128	1373.030	589.103	1953.271	-60.015
1800	1215.412	2235.937	1405.934	1494.006	591.621	2033.495	-59.009
1900	1225.533	2301.928	1451.368	1616.064	594.088	2113.511	-58.103
2000	1234.428	2365.021	1495.485	1739.072	596.441	2193.435	-57.285
2100	1242.279	2425.443	1538.340	1862.915	598.586	2273.228	-56.542
2200	1249.237	2483.397	1579.989	1987.498	600.526	2352.924	-55.864
2300	1255.428	2539.067	1620.486	2112.737	602.258	2432.540	-55.244
2400	1260.958	2592.617	1659.883	2238.561	603.694	2512.020	-54.672
2500	1265.914	2644.194	1698.230	2364.909	604.852	2591.594	-54.147
2600	1270.372	2693.932	1735.576	2491.728	605.688	2670.976	-53.659
2700	1274.393	2741.953	1771.965	2618.969	606.210	2750.430	-53.209
2800	1278.033	2788.367	1807.441	2746.594	606.385	2829.893	-52.791
2900	1281.336	2833.273	1842.044	2874.565	606.178	2909.290	-52.401
3000	1284.342	2876.764	1875.814	3002.851	605.647	2988.736	-52.037
3100	1287.085	2918.923	1908.786	3131.424	604.693	3068.102	-51.696
3200	1289.594	2959.826	1940.995	3260.260	603.370	3147.603	-51.378
3300	1291.894	2999.545	1972.473	3389.336	601.658	3227.205	-51.081
3400	1294.008	3038.144	2003.252	3518.633	599.519	3306.747	-50.801
3500	1295.955	3075.682	2033.359	3648.132	596.962	3386.335	-50.537
3600	1297.752	3112.216	2062.822	3777.819	594.015	3466.121	-50.291
3700	1299.414	3147.796	2091.667	3907.678	590.638	3546.010	-50.060
3800	1300.953	3182.470	2119.918	4037.697	586.801	3625.924	-49.841
3900	1302.381	3216.281	2147.598	4167.865	582.553	3705.871	-49.634
4000	1303.709	3249.272	2174.729	4298.170	577.877	3786.118	-49.441
4100	1304.945	3281.479	2201.332	4428.604	572.725	3866.390	-49.257
4200	1306.099	3312.939	2227.426	4559.157	567.135	3946.783	-49.084
4300	1307.176	3343.685	2253.029	4689.821	561.089	4027.195	-48.920
4400	1308.183	3373.748	2278.159	4820.589	554.599	4107.872	-48.766
4500	1309.127	3403.157	2302.834	4951.455	547.684	4188.772	-48.621
4600	1310.012	3431.940	2327.068	5082.413	540.275	4269.849	-48.485
4700	1310.844	3460.123	2350.877	5213.456	532.394	4350.940	-48.354
4800	1311.625	3487.729	2374.274	5344.580	524.099	4432.343	-48.233
4900	1312.361	3514.781	2397.275	5475.780	515.295	4513.744	-48.116
5000	1313.055	3541.301	2419.891	5607.051	506.103	4595.572	-48.009

3.643. Dibenzo[*rs,vwx*]naphtho[2,1,8,7-*klmn*]hexaphene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 117726-81-5
Point Group: C₁

Length: 18.04 Å
Width: 11.62 Å
Breadth: 5.004 Å
L/B Ratio: 1.552

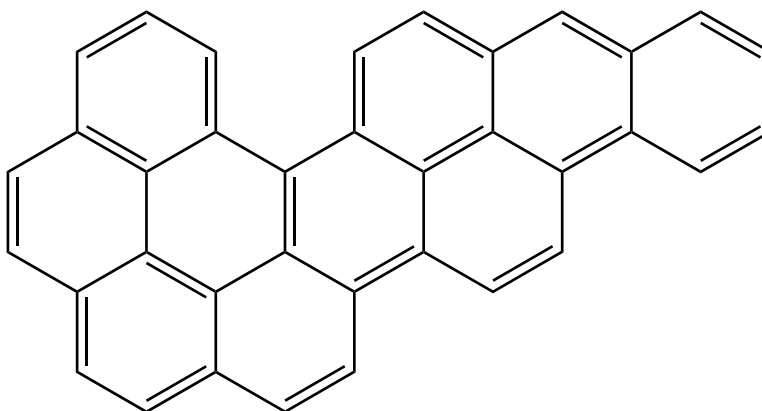
Cartesian coordinates:

C	-1.2391	-0.6797	-0.0840	C	4.9481	-2.4674	0.3849	H	0.3596	2.9417	-0.9730
C	-0.6446	-1.9471	-0.2370	C	5.7474	-1.3603	0.4974	H	1.8785	4.8571	-1.1102
C	0.7587	-2.0647	-0.1593	C	1.3879	-3.3560	-0.1383	H	4.2780	4.6291	-0.4899
C	1.5571	-0.8998	-0.0831	C	2.7249	-3.4912	0.0264	H	6.1510	3.2224	0.1951
C	0.9693	0.3908	-0.1084	C	-2.6735	-0.5745	-0.0478	H	7.0985	0.9660	0.6288
C	-0.4329	0.4863	0.0370	C	-3.4813	-1.7372	-0.2496	H	6.8234	-1.4647	0.6779
C	2.9798	-1.0582	0.0671	C	-2.8287	-3.0075	-0.4550	H	5.3757	-3.4731	0.4694
C	3.8177	0.0864	0.1507	C	-1.4837	-3.1037	-0.4360	H	3.1945	-4.4807	0.0619
C	3.2539	1.3866	-0.0546	C	-3.2891	0.6586	0.1903	H	0.7431	-4.2413	-0.2481
C	1.8572	1.5439	-0.2730	C	-4.7132	0.7597	0.2105	H	-0.9851	-4.0752	-0.5738
C	4.1171	2.5007	-0.1023	C	-5.4915	-0.3956	-0.0138	H	-3.4578	-3.8901	-0.6182
C	3.6076	3.7631	-0.4556	C	-4.8567	-1.6403	-0.2389	H	-5.4750	-2.5319	-0.4021
C	2.2753	3.8895	-0.7849	C	-6.9110	-0.2936	-0.0039	H	-7.5056	-1.1968	-0.1821
C	1.4129	2.7922	-0.6990	C	-7.5174	0.9107	0.2245	H	-8.6091	0.9933	0.2320
C	5.1957	-0.0633	0.3651	C	-6.7388	2.0691	0.4562	H	-7.2446	3.0226	0.6404
C	6.0320	1.0996	0.4146	C	-5.3731	1.9960	0.4502	H	-4.7521	2.8866	0.6316
C	5.5139	2.3306	0.1806	C	-1.1097	1.7135	0.3599	H	-2.9580	2.7480	0.6861
C	3.5564	-2.3325	0.1597	C	-2.4588	1.7996	0.4328	H	-0.5054	2.6065	0.5717

Table 3.643: Table of thermodynamic data as a function of temperature for Dibenz[rs,vwx]naphtho[2,1,8,7-klmn]hexaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-62.686	574.472	574.472	∞
100	131.605	379.246	928.634	-54.939	604.421	660.578	-345.043
200	275.384	512.323	686.912	-34.918	588.460	723.128	-188.858
250	357.233	582.518	658.970	-19.113	581.045	757.651	-158.299
298.15	436.402	652.230	652.230	0.000	574.472	792.279	-138.801
300	439.401	654.939	652.238	0.810	574.229	793.628	-138.180
350	518.175	728.650	657.880	24.770	568.192	830.687	-123.971
400	591.187	802.682	671.355	52.531	562.968	868.540	-113.417
450	657.342	876.202	690.039	83.774	558.453	907.013	-105.281
500	716.483	948.581	712.286	118.148	554.542	945.984	-98.824
600	815.579	1088.333	763.417	194.949	548.174	1024.903	-89.224
700	893.716	1220.156	819.348	280.566	543.520	1104.757	-82.436
800	956.097	1343.718	877.257	373.169	540.391	1185.151	-77.381
900	1006.666	1459.350	935.581	471.392	538.588	1265.847	-73.466
1000	1048.223	1567.633	993.430	574.203	537.935	1346.697	-70.343
1100	1082.761	1669.209	1050.296	680.804	538.201	1427.581	-67.789
1200	1111.731	1764.699	1105.891	790.570	539.229	1508.381	-65.657
1300	1136.219	1854.679	1160.063	903.001	540.807	1589.086	-63.849
1400	1157.063	1939.665	1212.742	1017.692	542.782	1669.659	-62.294
1500	1174.915	2020.118	1263.909	1134.314	545.068	1750.083	-60.942
1600	1190.293	2096.449	1313.578	1252.593	547.508	1830.335	-59.753
1700	1203.611	2169.019	1361.781	1372.304	550.021	1910.403	-58.698
1800	1215.205	2238.151	1408.564	1493.258	552.517	1990.405	-57.759
1900	1225.346	2304.132	1453.976	1615.296	554.963	2070.201	-56.913
2000	1234.259	2367.215	1498.072	1738.286	557.299	2149.905	-56.149
2100	1242.124	2427.629	1540.908	1862.113	559.428	2229.478	-55.454
2200	1249.096	2485.577	1582.540	1986.681	561.353	2308.957	-54.820
2300	1255.299	2541.241	1623.020	2111.907	563.072	2388.355	-54.240
2400	1260.839	2594.785	1662.402	2237.719	564.495	2467.618	-53.705
2500	1265.804	2646.358	1700.735	2364.055	565.641	2546.975	-53.215
2600	1270.270	2696.092	1738.068	2490.863	566.467	2626.141	-52.759
2700	1274.299	2744.109	1774.444	2618.095	566.979	2705.379	-52.338
2800	1277.945	2790.519	1809.908	2745.710	567.145	2784.627	-51.947
2900	1281.254	2835.423	1844.501	2873.673	566.930	2863.809	-51.582
3000	1284.265	2878.911	1878.260	3001.951	566.391	2943.040	-51.242
3100	1287.013	2921.067	1911.223	3130.517	565.429	3022.191	-50.923
3200	1289.526	2961.968	1943.423	3259.346	564.100	3101.478	-50.625
3300	1291.831	3001.685	1974.892	3388.415	562.381	3180.865	-50.348
3400	1293.949	3040.282	2005.662	3517.706	560.236	3260.193	-50.086
3500	1295.899	3077.819	2035.762	3647.199	557.672	3339.568	-49.839
3600	1297.699	3114.351	2065.217	3776.880	554.720	3419.140	-49.609
3700	1299.363	3149.929	2094.055	3906.735	551.339	3498.816	-49.393
3800	1300.905	3184.602	2122.300	4036.749	547.496	3578.517	-49.189
3900	1302.335	3218.412	2149.973	4166.912	543.244	3658.251	-48.996
4000	1303.666	3251.402	2177.098	4297.213	538.563	3738.285	-48.816
4100	1304.904	3283.608	2203.695	4427.642	533.407	3818.344	-48.645
4200	1306.059	3315.067	2229.783	4558.191	527.813	3898.523	-48.484
4300	1307.138	3345.812	2255.381	4688.851	521.763	3978.723	-48.331
4400	1308.147	3375.874	2280.507	4819.616	515.269	4059.187	-48.188
4500	1309.093	3405.283	2305.176	4950.479	508.351	4139.875	-48.053
4600	1309.979	3434.065	2329.406	5081.433	500.939	4220.739	-47.927
4700	1310.812	3462.246	2353.210	5212.473	493.055	4301.617	-47.806
4800	1311.595	3489.852	2376.603	5343.593	484.756	4382.808	-47.694
4900	1312.333	3516.904	2399.600	5474.790	475.949	4463.997	-47.586
5000	1313.027	3543.423	2422.212	5606.059	466.755	4545.613	-47.487

3.644. Benzo[*rst*]pyreno[1,10,9-*cde*]pentaphene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 117740-28-0
Point Group: C₁

Length: 18.36 Å
Width: 11.84 Å
Breadth: 5.054 Å
L/B Ratio: 1.551

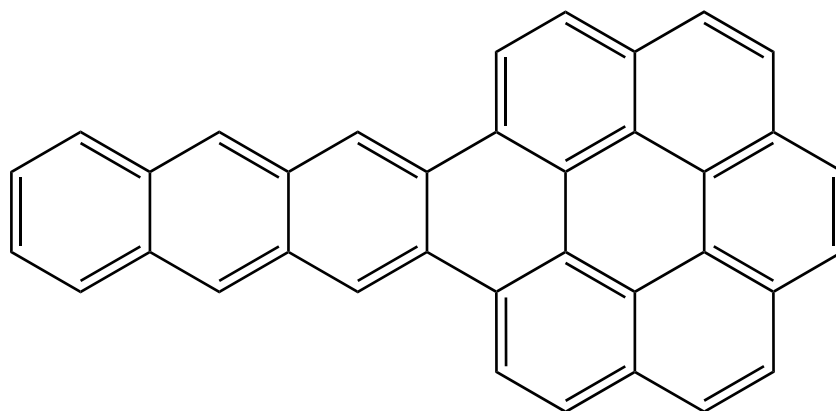
Cartesian coordinates:

C	6.7478	-1.3102	0.2116	C	-2.1694	-1.5115	-0.2279	H	-0.9175	-3.1633	-0.8481
C	5.3772	-0.9417	0.1835	C	-3.5239	-1.1071	-0.0605	H	-2.7429	-4.7880	-1.0097
C	5.0243	0.3999	-0.0635	C	-3.8587	0.2753	0.1047	H	-5.0846	-4.1310	-0.4805
C	6.0550	1.3510	-0.2750	C	-2.8299	1.2570	0.0322	H	-6.7027	-2.4048	0.1135
C	7.3723	0.9746	-0.2435	C	-4.5660	-2.0541	-0.1209	H	-7.2544	-0.0088	0.4798
C	7.7228	-0.3705	0.0017	C	-4.2737	-3.3953	-0.4364	H	-6.5635	2.3351	0.5049
C	3.6382	0.7698	-0.0968	C	-2.9761	-3.7590	-0.7158	H	-4.7837	4.0591	0.3170
C	2.6497	-0.2025	0.1017	C	-1.9370	-2.8254	-0.6168	H	-2.4463	4.6632	-0.0221
C	3.0363	-1.5554	0.3703	C	-5.1935	0.6658	0.2687	H	-0.0629	3.9905	-0.2407
C	4.3619	-1.9107	0.4074	C	-6.2212	-0.3305	0.3061	H	1.6260	3.5143	-0.5023
C	1.2602	0.1477	0.0388	C	-5.9189	-1.6385	0.1089	H	4.0355	2.8704	-0.4835
C	0.9061	1.4917	-0.1566	C	-3.1788	2.6144	0.0865	H	4.6549	-2.9476	0.6140
C	1.9304	2.4686	-0.3438	C	-4.5366	2.9926	0.2619	H	2.2940	-3.5326	0.9224
C	3.2443	2.1211	-0.3273	C	-5.5163	2.0449	0.3629	H	-0.0747	-2.9440	0.7429
C	0.2484	-0.8600	0.1511	C	-0.8575	3.2345	-0.1462	H	5.7669	2.3963	-0.4649
C	-1.0948	-0.5298	-0.0503	C	-2.1587	3.6057	-0.0307	H	8.1644	1.7123	-0.4080
C	-1.4555	0.8566	-0.0710	C	0.6923	-2.1888	0.5206	H	8.7807	-0.6519	0.0224
C	-0.4719	1.8572	-0.1334	C	1.9925	-2.5209	0.6261	H	7.0111	-2.3565	0.4037

Table 3.644: Table of thermodynamic data as a function of temperature for Benzo[*rst*]pyreno[1,10,9-*cde*]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-62.846	572.044	572.044	∞
100	132.163	381.907	932.080	-55.017	601.915	657.805	-343.595
200	275.759	515.294	690.057	-34.953	585.997	720.071	-188.059
250	357.583	585.570	662.089	-19.130	578.600	754.444	-157.629
298.15	436.742	655.343	655.343	0.000	572.044	788.923	-138.213
300	439.741	658.054	655.351	0.811	571.802	790.267	-137.595
350	518.508	731.817	660.997	24.787	565.781	827.168	-123.446
400	591.511	805.893	674.481	52.565	560.574	864.862	-112.937
450	657.654	879.451	693.177	83.823	556.075	903.174	-104.835
500	716.780	951.862	715.436	118.213	552.179	941.980	-98.406
600	815.841	1091.665	766.594	195.043	545.839	1020.569	-88.847
700	893.943	1223.525	822.550	280.683	541.210	1100.088	-82.088
800	956.291	1347.115	880.481	373.307	538.101	1180.143	-77.054
900	1006.833	1462.769	938.826	471.549	536.317	1260.498	-73.156
1000	1048.368	1571.068	996.693	574.375	535.679	1341.006	-70.046
1100	1082.887	1672.657	1053.575	680.989	535.958	1421.546	-67.502
1200	1111.840	1768.157	1109.185	790.767	536.998	1502.000	-65.379
1300	1136.316	1858.145	1163.370	903.208	538.586	1582.360	-63.579
1400	1157.148	1943.138	1216.060	1017.909	540.571	1662.585	-62.031
1500	1174.991	2023.597	1267.238	1134.538	542.864	1742.662	-60.684
1600	1190.361	2099.932	1316.917	1252.825	545.312	1822.566	-59.499
1700	1203.672	2172.506	1365.128	1372.542	547.831	1902.285	-58.449
1800	1215.260	2241.642	1411.918	1493.502	550.333	1981.938	-57.513
1900	1225.397	2307.625	1457.338	1615.546	552.785	2061.385	-56.670
2000	1234.304	2370.711	1501.441	1738.540	555.125	2140.739	-55.909
2100	1242.166	2431.127	1544.283	1862.372	557.259	2219.963	-55.217
2200	1249.134	2489.077	1585.920	1986.944	559.188	2299.091	-54.586
2300	1255.334	2544.742	1626.406	2112.173	560.910	2378.139	-54.008
2400	1260.872	2598.288	1665.793	2237.988	562.336	2457.052	-53.475
2500	1265.835	2649.862	1704.130	2364.328	563.486	2536.059	-52.987
2600	1270.298	2699.597	1741.467	2491.139	564.315	2614.875	-52.532
2700	1274.325	2747.615	1777.847	2618.373	564.829	2693.762	-52.113
2800	1277.969	2794.027	1813.315	2745.991	564.998	2772.659	-51.724
2900	1281.277	2838.931	1847.911	2873.956	564.785	2851.491	-51.360
3000	1284.287	2882.420	1881.674	3002.236	564.248	2930.371	-51.021
3100	1287.033	2924.577	1914.640	3130.804	563.288	3009.171	-50.703
3200	1289.545	2965.478	1946.842	3259.635	561.961	3088.107	-50.407
3300	1291.849	3005.196	1978.315	3388.707	560.245	3167.143	-50.131
3400	1293.965	3043.793	2009.088	3517.999	558.101	3246.120	-49.870
3500	1295.915	3081.330	2039.189	3647.494	555.539	3325.144	-49.624
3600	1297.714	3117.863	2068.647	3777.177	552.589	3404.365	-49.395
3700	1299.377	3153.442	2097.487	3907.032	549.208	3483.689	-49.180
3800	1300.918	3188.115	2125.734	4037.048	545.367	3563.039	-48.976
3900	1302.348	3221.926	2153.410	4167.212	541.116	3642.421	-48.784
4000	1303.678	3254.915	2180.537	4297.514	536.436	3722.104	-48.605
4100	1304.916	3287.122	2207.135	4427.945	531.282	3801.812	-48.435
4200	1306.070	3318.581	2233.225	4558.495	525.689	3881.640	-48.274
4300	1307.149	3349.326	2258.825	4689.156	519.640	3961.488	-48.122
4400	1308.158	3379.389	2283.952	4819.922	513.147	4041.601	-47.979
4500	1309.103	3408.797	2308.623	4950.786	506.230	4121.937	-47.845
4600	1309.989	3437.580	2332.854	5081.741	498.819	4202.450	-47.719
4700	1310.821	3465.762	2356.659	5212.782	490.936	4282.977	-47.599
4800	1311.604	3493.367	2380.054	5343.903	482.638	4363.816	-47.487
4900	1312.341	3520.419	2403.052	5475.101	473.832	4444.653	-47.380
5000	1313.035	3546.939	2425.665	5606.370	464.638	4525.917	-47.281

3.645. Anthra[2,3-*a*]coronene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 5869-17-0
Point Group: C_{2v}

Length: 18.99 Å
Width: 11.66 Å
Breadth: 3.885 Å
L/B Ratio: 1.629

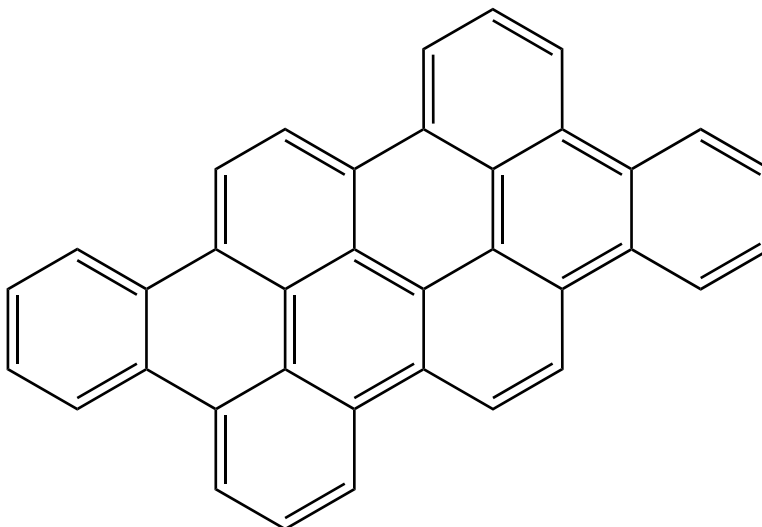
Cartesian coordinates:

C	0.2724	2.8479	0.0000	C	0.2384	-1.4339	0.0000	H	-0.6841	3.3932	0.0000
C	1.4620	3.5324	0.0000	C	1.4401	-0.7229	0.0000	H	1.4724	4.6283	0.0000
C	2.6891	2.8318	0.0000	C	1.4400	0.7231	0.0000	H	6.0764	3.3719	0.0000
C	2.6757	1.4261	0.0000	C	0.2382	1.4340	0.0000	H	3.9297	4.6202	0.0000
C	5.1175	2.8410	0.0000	C	-1.0308	-0.7183	0.0000	H	7.2971	-1.2406	0.0000
C	3.9422	3.5242	0.0000	C	-1.0309	0.7182	0.0000	H	7.2970	1.2416	0.0000
C	5.1322	1.4101	0.0000	C	-2.2282	1.3969	0.0000	H	3.9303	-4.6196	0.0000
C	3.9173	0.7122	0.0000	C	-2.2280	-1.3972	0.0000	H	6.0769	-3.3710	0.0000
C	6.3530	-0.6838	0.0000	C	-3.4713	-0.7105	0.0000	H	-0.6837	-3.3932	0.0000
C	6.3530	0.6847	0.0000	C	-3.4714	0.7101	0.0000	H	1.4730	-4.6281	0.0000
C	5.1324	-1.4094	0.0000	C	-4.6912	1.4049	0.0000	H	-2.2297	2.4990	0.0000
C	3.9174	-0.7116	0.0000	C	-4.6910	-1.4056	0.0000	H	-2.2293	-2.4993	0.0000
C	3.9427	-3.5236	0.0000	C	-5.8976	-0.7132	0.0000	H	-4.6891	2.5018	0.0000
C	5.1179	-2.8404	0.0000	C	-5.8977	0.7124	0.0000	H	-4.6887	-2.5025	0.0000
C	2.6894	-2.8314	0.0000	C	-7.1558	1.4045	0.0000	H	-7.1459	2.5004	0.0000
C	2.6759	-1.4257	0.0000	C	-8.3248	0.7133	0.0000	H	-9.2865	1.2365	0.0000
C	0.2728	-2.8479	0.0000	C	-8.3247	-0.7145	0.0000	H	-9.2863	-1.2379	0.0000
C	1.4624	-3.5322	0.0000	C	-7.1556	-1.4056	0.0000	H	-7.1455	-2.5014	0.0000

Table 3.645: Table of thermodynamic data as a function of temperature for Anthra[2,3-*a*]coronene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _f
0	0.0	0.0	∞	-62.679	541.801	541.801	∞
100	131.794	375.974	924.593	-54.862	571.827	628.311	-328.189
200	274.918	508.897	683.231	-34.867	555.840	691.193	-180.517
250	356.713	578.982	655.329	-19.087	548.400	725.891	-151.663
298.15	435.825	648.598	648.598	0.000	541.801	760.691	-133.267
300	438.821	651.303	648.606	0.809	541.557	762.047	-132.681
350	517.525	724.920	654.240	24.738	535.489	799.290	-119.285
400	590.476	798.860	667.698	52.465	530.231	837.331	-109.342
450	656.596	872.295	686.359	83.671	525.680	875.998	-101.681
500	715.731	944.595	708.579	118.008	521.731	915.166	-95.605
600	814.882	1084.213	759.652	194.736	515.290	994.491	-86.576
700	893.124	1215.936	815.525	280.288	510.572	1074.762	-80.198
800	955.622	1339.427	873.379	372.838	507.389	1155.582	-75.450
900	1006.301	1455.009	931.654	471.020	505.544	1236.709	-71.775
1000	1047.951	1563.259	989.461	573.798	504.859	1317.996	-68.844
1100	1082.564	1664.812	1046.289	680.376	505.102	1399.318	-66.447
1200	1111.592	1760.288	1101.851	790.125	506.113	1480.558	-64.446
1300	1136.125	1850.259	1155.994	902.545	507.679	1561.706	-62.749
1400	1157.003	1935.239	1208.647	1017.229	509.647	1642.720	-61.289
1500	1174.881	2015.689	1259.792	1133.845	511.928	1723.587	-60.019
1600	1190.278	2092.018	1309.442	1252.122	514.366	1804.283	-58.903
1700	1203.610	2164.588	1357.628	1371.832	516.878	1884.794	-57.911
1800	1215.214	2233.720	1404.394	1492.787	519.374	1965.239	-57.029
1900	1225.363	2299.701	1449.793	1614.827	521.822	2045.477	-56.233
2000	1234.281	2362.786	1493.877	1737.818	524.160	2125.624	-55.514
2100	1242.151	2423.201	1536.702	1861.648	526.292	2205.641	-54.861
2200	1249.125	2481.150	1578.323	1986.219	528.219	2285.562	-54.265
2300	1255.329	2536.815	1618.795	2111.447	529.941	2365.402	-53.719
2400	1260.870	2590.361	1658.168	2237.262	531.367	2445.108	-53.215
2500	1265.836	2641.935	1696.494	2363.602	532.517	2524.908	-52.754
2600	1270.302	2691.670	1733.819	2490.413	533.346	2604.516	-52.324
2700	1274.331	2739.689	1770.189	2617.648	533.861	2684.196	-51.928
2800	1277.976	2786.100	1805.648	2745.266	534.030	2763.886	-51.560
2900	1281.285	2831.004	1840.235	2873.232	533.818	2843.510	-51.216
3000	1284.295	2874.493	1873.989	3001.513	533.282	2923.183	-50.896
3100	1287.042	2916.651	1906.947	3130.082	532.323	3002.776	-50.595
3200	1289.555	2957.553	1939.142	3258.914	530.997	3082.504	-50.316
3300	1291.858	2997.270	1970.608	3387.986	529.281	3162.333	-50.055
3400	1293.975	3035.868	2001.374	3517.279	527.138	3242.102	-49.808
3500	1295.925	3073.406	2031.470	3646.776	524.577	3321.918	-49.576
3600	1297.724	3109.939	2060.922	3776.459	521.628	3401.932	-49.360
3700	1299.387	3145.518	2089.757	3906.316	518.249	3482.049	-49.157
3800	1300.928	3180.191	2117.998	4036.333	514.408	3562.191	-48.965
3900	1302.358	3214.002	2145.669	4166.498	510.159	3642.366	-48.783
4000	1303.687	3246.992	2172.792	4296.801	505.480	3722.840	-48.614
4100	1304.925	3279.199	2199.386	4427.232	500.326	3803.341	-48.454
4200	1306.080	3310.658	2225.472	4557.783	494.734	3883.961	-48.303
4300	1307.158	3341.404	2251.067	4688.446	488.686	3964.601	-48.159
4400	1308.166	3371.466	2276.191	4819.212	482.194	4045.507	-48.025
4500	1309.111	3400.875	2300.858	4950.077	475.278	4126.635	-47.900
4600	1309.997	3429.658	2325.086	5081.033	467.867	4207.940	-47.782
4700	1310.829	3457.840	2348.888	5212.074	459.985	4289.259	-47.669
4800	1311.612	3485.446	2372.280	5343.197	451.689	4370.890	-47.564
4900	1312.349	3512.498	2395.274	5474.395	442.883	4452.520	-47.463
5000	1313.043	3539.018	2417.885	5605.665	433.690	4534.576	-47.371

3.646. Dibenzo[*ij,rst*]phenanthro[9,10,1,2-*defg*]pentaphene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 313-65-5
Point Group: C_{2h}

Length: 18.06 Å
Width: 10.41 Å
Breadth: 3.890 Å
L/B Ratio: 1.735

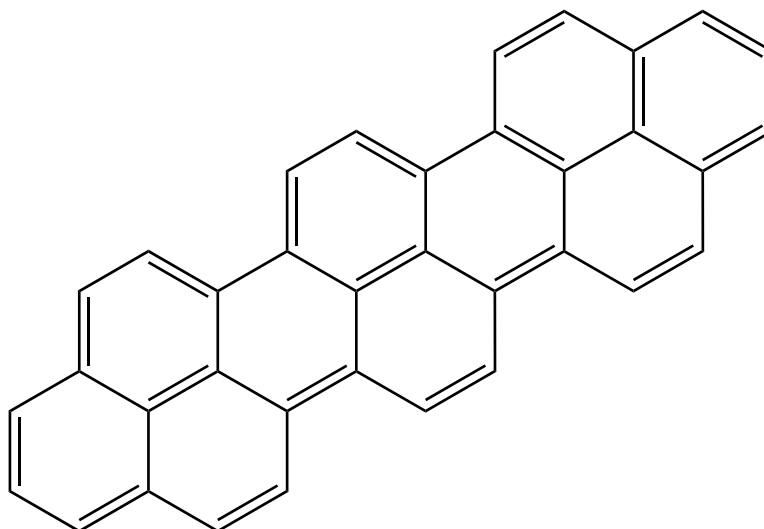
Cartesian coordinates:

C	4.1607	2.6835	0.0000	C	5.1449	-2.1231	0.0000	H	5.2423	2.8881	0.0000
C	3.2513	3.7305	0.0000	C	6.5010	-1.8654	0.0000	H	3.6087	4.7655	0.0000
C	1.8882	3.4688	0.0000	C	6.9605	-0.5445	0.0000	H	1.1654	4.2988	0.0000
C	3.7204	1.3556	0.0000	C	6.0570	0.4992	0.0000	H	0.5831	-3.9612	0.0000
C	2.7817	-1.3437	0.0000	C	-1.4143	-2.1535	0.0000	H	3.0258	-3.4925	0.0000
C	0.9484	-2.9227	0.0000	C	-4.1607	-2.6835	0.0000	H	-0.5831	3.9612	0.0000
C	2.3017	-2.6632	0.0000	C	-3.2513	-3.7305	0.0000	H	-3.0257	3.4925	0.0000
C	0.0136	-1.8747	0.0000	C	-1.8883	-3.4688	0.0000	H	4.7754	-3.1600	0.0000
C	-0.9483	2.9226	0.0000	C	-2.3354	-1.0836	0.0000	H	7.2188	-2.6920	0.0000
C	-2.3017	2.6632	0.0000	C	-1.8633	0.2795	0.0000	H	8.0364	-0.3418	0.0000
C	2.3354	1.0836	0.0000	C	-2.7817	1.3437	0.0000	H	6.4104	1.5417	0.0000
C	1.4143	2.1535	0.0000	C	-3.7204	-1.3556	0.0000	H	-5.2423	-2.8881	0.0000
C	-0.0136	1.8746	0.0000	C	-4.6716	-0.2549	0.0000	H	-3.6088	-4.7655	0.0000
C	-0.4715	0.5466	0.0000	C	-4.2099	1.0716	0.0000	H	-1.1654	-4.2989	0.0000
C	0.4715	-0.5466	0.0000	C	-5.1449	2.1231	0.0000	H	-4.7754	3.1600	0.0000
C	1.8633	-0.2795	0.0000	C	-6.5010	1.8654	0.0000	H	-7.2188	2.6921	0.0000
C	4.6715	0.2549	0.0000	C	-6.9605	0.5446	0.0000	H	-8.0364	0.3419	0.0000
C	4.2099	-1.0716	0.0000	C	-6.0570	-0.4991	0.0000	H	-6.4105	-1.5416	0.0000

Table 3.646: Table of thermodynamic data as a function of temperature for Dibenzo[*ij,rst*]phenanthro[9,10,1,2-*defg*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-63.798	537.488	537.488	∞
100	137.645	396.028	949.203	-55.318	567.058	621.537	-324.651
200	276.864	531.835	706.482	-34.929	551.464	682.229	-178.176
250	357.221	602.187	678.550	-19.091	544.083	715.772	-149.549
298.15	435.573	671.820	671.820	0.000	537.488	749.454	-131.299
300	438.550	674.523	671.828	0.809	537.243	750.767	-130.717
350	516.936	748.070	677.457	24.714	531.152	786.850	-117.429
400	589.816	821.925	690.901	52.410	525.862	823.737	-107.567
450	655.967	895.283	709.543	83.583	521.279	861.252	-99.970
500	715.159	967.520	731.740	117.890	517.300	899.272	-93.944
600	814.386	1107.042	782.765	194.566	510.806	976.310	-84.994
700	892.625	1238.689	838.592	280.068	506.039	1054.302	-78.671
800	955.074	1362.110	896.403	372.566	502.804	1132.850	-73.966
900	1005.694	1477.625	954.636	470.690	500.901	1211.712	-70.325
1000	1047.296	1585.808	1012.403	573.405	500.153	1290.741	-67.420
1100	1081.877	1687.297	1069.192	679.916	500.328	1369.811	-65.046
1200	1110.891	1782.713	1124.716	789.595	501.270	1448.806	-63.064
1300	1135.425	1872.627	1178.823	901.945	502.766	1527.714	-61.383
1400	1156.314	1957.556	1231.442	1016.559	504.665	1606.494	-59.938
1500	1174.211	2037.959	1282.554	1133.108	506.878	1685.132	-58.680
1600	1189.633	2114.245	1332.171	1251.319	509.250	1763.602	-57.575
1700	1202.993	2186.777	1380.326	1370.966	511.698	1841.893	-56.593
1800	1214.626	2255.875	1427.064	1491.860	514.135	1920.120	-55.719
1900	1224.805	2321.825	1472.434	1613.843	516.525	1998.145	-54.932
2000	1233.751	2384.882	1516.492	1736.780	518.808	2076.081	-54.221
2100	1241.649	2445.272	1559.292	1860.558	520.889	2153.889	-53.574
2200	1248.651	2503.198	1600.889	1985.080	522.767	2231.604	-52.984
2300	1254.881	2558.843	1641.337	2110.262	524.443	2309.241	-52.443
2400	1260.447	2612.370	1680.689	2236.034	525.825	2386.745	-51.945
2500	1265.436	2663.927	1718.994	2362.333	526.934	2464.345	-51.489
2600	1269.923	2713.647	1756.299	2489.104	527.724	2541.754	-51.063
2700	1273.972	2761.651	1792.650	2616.303	528.202	2619.238	-50.671
2800	1277.636	2808.050	1828.091	2743.886	528.337	2696.732	-50.307
2900	1280.963	2852.943	1862.661	2871.819	528.091	2774.161	-49.967
3000	1283.990	2896.421	1896.399	3000.069	527.524	2851.641	-49.650
3100	1286.752	2938.569	1929.341	3128.608	526.535	2929.042	-49.353
3200	1289.279	2979.462	1961.521	3257.411	525.181	3006.579	-49.076
3300	1291.596	3019.171	1992.972	3386.457	523.438	3084.217	-48.818
3400	1293.726	3057.761	2023.725	3515.724	521.270	3161.797	-48.574
3500	1295.687	3095.292	2053.807	3645.196	518.685	3239.424	-48.345
3600	1297.497	3131.818	2083.247	3774.857	515.712	3317.249	-48.131
3700	1299.171	3167.392	2112.070	3904.691	512.311	3395.178	-47.930
3800	1300.722	3202.059	2140.299	4034.687	508.449	3473.133	-47.741
3900	1302.161	3235.865	2167.959	4164.832	504.179	3551.121	-47.561
4000	1303.499	3268.850	2195.071	4295.115	499.481	3629.410	-47.394
4100	1304.744	3301.052	2221.655	4425.528	494.309	3707.725	-47.236
4200	1305.906	3332.507	2247.731	4556.062	488.699	3786.160	-47.087
4300	1306.992	3363.249	2273.317	4686.707	482.635	3864.616	-46.945
4400	1308.007	3393.308	2298.431	4817.458	476.126	3943.337	-46.812
4500	1308.958	3422.713	2323.089	4948.306	469.194	4022.281	-46.688
4600	1309.850	3451.492	2347.308	5079.247	461.769	4101.402	-46.572
4700	1310.688	3479.671	2371.102	5210.275	453.872	4180.538	-46.461
4800	1311.476	3507.274	2394.486	5341.383	445.562	4259.987	-46.357
4900	1312.218	3534.324	2417.473	5472.568	436.743	4339.433	-46.258
5000	1312.917	3560.841	2440.076	5603.825	427.537	4419.307	-46.167

3.647. Benzo[*rst*]dinaphtho[8,1,2-*cde*:2',1',8'-*klm*]pentaphene



Formula: C₃₆H₁₈
Mass: 450.528 g/mol
CAS Number: 56181-09-0
Point Group: D_{2h}

Length: 20.12 Å
Width: 9.199 Å
Breadth: 3.884 Å
L/B Ratio: 2.188

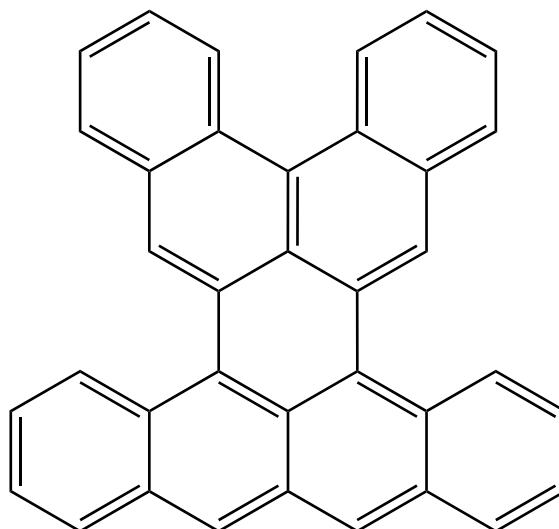
Cartesian coordinates:

C	7.0777	-1.2136	0.0000	C	-1.4257	-1.2251	0.0000	H	7.6284	-2.1612	0.0000
C	7.7667	-0.0071	0.0000	C	-0.6782	-2.4529	0.0000	H	8.8619	-0.0080	0.0000
C	7.0798	1.2007	0.0000	C	0.6736	-2.4542	0.0000	H	7.6324	2.1471	0.0000
C	5.6817	1.2161	0.0000	C	1.4235	-1.2278	0.0000	H	5.5083	3.3908	0.0000
C	4.9436	2.4514	0.0000	C	0.7192	-0.0007	0.0000	H	3.0246	3.3949	0.0000
C	3.5913	2.4511	0.0000	C	-2.8330	1.2305	0.0000	H	3.0185	-3.4005	0.0000
C	2.8352	1.2253	0.0000	C	-3.5868	2.4577	0.0000	H	5.5021	-3.4009	0.0000
C	3.5339	-0.0033	0.0000	C	-4.9391	2.4605	0.0000	H	1.2464	3.3957	0.0000
C	2.8330	-1.2306	0.0000	C	-5.6795	1.2266	0.0000	H	-1.2402	3.3980	0.0000
C	3.5868	-2.4577	0.0000	C	-7.0776	1.2137	0.0000	H	-1.2464	-3.3957	0.0000
C	4.9392	-2.4605	0.0000	C	-7.7667	0.0071	0.0000	H	1.2402	-3.3980	0.0000
C	5.6795	-1.2265	0.0000	C	-7.0799	-1.2007	0.0000	H	-3.0183	3.4005	0.0000
C	4.9690	-0.0046	0.0000	C	-4.9690	0.0046	0.0000	H	-5.5021	3.4009	0.0000
C	1.4258	1.2251	0.0000	C	-5.6817	-1.2161	0.0000	H	-7.6284	2.1611	0.0000
C	0.6781	2.4529	0.0000	C	-4.9437	-2.4514	0.0000	H	-8.8619	0.0083	0.0000
C	-0.6736	2.4541	0.0000	C	-3.5913	-2.4511	0.0000	H	-7.6323	-2.1471	0.0000
C	-1.4235	1.2277	0.0000	C	-2.8353	-1.2253	0.0000	H	-5.5083	-3.3908	0.0000
C	-0.7192	0.0006	0.0000	C	-3.5339	0.0032	0.0000	H	-3.0247	-3.3949	0.0000

Table 3.647: Table of thermodynamic data as a function of temperature for Benzo[*rst*]dinaphtho[8,1,2-*cde*:2',1',8'-*klm*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-63.086	558.783	558.783	∞
100	133.257	373.417	924.805	-55.139	588.532	645.272	-337.048
200	276.311	507.336	682.338	-35.000	572.688	708.353	-184.999
250	358.071	577.728	654.335	-19.152	565.317	743.121	-155.263
298.15	437.164	647.581	647.581	0.000	558.783	777.976	-136.295
300	440.160	650.295	647.590	0.812	558.541	779.334	-135.691
350	518.859	724.118	653.240	24.807	552.540	816.622	-121.872
400	591.801	798.236	666.734	52.601	547.348	854.699	-111.610
450	657.892	871.825	685.442	83.872	542.863	893.393	-103.700
500	716.975	944.259	707.713	118.273	538.978	932.581	-97.424
600	815.971	1084.091	758.894	195.119	532.654	1011.928	-88.094
700	894.026	1215.968	814.869	280.770	528.035	1092.203	-81.499
800	956.340	1339.567	872.816	373.401	524.933	1173.014	-76.588
900	1006.856	1455.225	931.174	471.646	523.152	1254.124	-72.786
1000	1048.373	1563.526	989.053	574.473	522.515	1335.386	-69.752
1100	1082.879	1665.114	1045.944	681.087	522.795	1416.679	-67.271
1200	1111.823	1760.613	1101.561	790.863	523.833	1497.888	-65.200
1300	1136.293	1850.600	1155.752	903.303	525.419	1579.002	-63.444
1400	1157.122	1935.591	1208.447	1018.001	527.402	1659.982	-61.933
1500	1174.962	2016.048	1259.629	1134.628	529.692	1740.814	-60.619
1600	1190.331	2092.381	1309.311	1252.911	532.137	1821.473	-59.464
1700	1203.642	2164.953	1357.526	1372.625	534.653	1901.948	-58.439
1800	1215.230	2234.087	1404.319	1493.582	537.152	1982.356	-57.525
1900	1225.367	2300.069	1449.741	1615.623	539.601	2062.558	-56.702
2000	1234.276	2363.153	1493.846	1738.615	541.938	2142.668	-55.960
2100	1242.139	2423.568	1536.690	1862.443	544.069	2222.648	-55.284
2200	1249.108	2481.516	1578.329	1987.013	545.995	2302.532	-54.668
2300	1255.309	2537.181	1618.816	2112.239	547.715	2382.336	-54.103
2400	1260.847	2590.725	1658.203	2238.052	549.139	2462.006	-53.583
2500	1265.812	2642.298	1696.542	2364.390	550.286	2541.769	-53.106
2600	1270.276	2692.033	1733.880	2491.198	551.113	2621.340	-52.662
2700	1274.304	2740.050	1770.261	2618.430	551.625	2700.984	-52.253
2800	1277.949	2786.460	1805.730	2746.046	551.792	2780.638	-51.872
2900	1281.258	2831.364	1840.326	2874.009	551.577	2860.226	-51.517
3000	1284.268	2874.852	1874.090	3002.288	551.038	2939.863	-51.187
3100	1287.016	2917.009	1907.056	3130.854	550.077	3019.420	-50.876
3200	1289.529	2957.910	1939.259	3259.683	548.748	3099.113	-50.587
3300	1291.833	2997.627	1970.732	3388.753	547.029	3178.906	-50.317
3400	1293.950	3036.223	2001.505	3518.043	544.884	3258.640	-50.062
3500	1295.900	3073.760	2031.607	3647.537	542.321	3338.420	-49.822
3600	1297.700	3110.293	2061.065	3777.218	539.369	3418.398	-49.599
3700	1299.364	3145.871	2089.906	3907.073	535.987	3498.480	-49.389
3800	1300.906	3180.544	2118.152	4037.087	532.145	3578.587	-49.190
3900	1302.336	3214.354	2145.829	4167.250	527.893	3658.726	-49.002
4000	1303.666	3247.343	2172.956	4297.551	523.212	3739.166	-48.827
4100	1304.905	3279.550	2199.555	4427.980	518.056	3819.631	-48.662
4200	1306.060	3311.009	2225.645	4558.529	512.462	3900.216	-48.505
4300	1307.139	3341.754	2251.245	4689.190	506.412	3980.822	-48.356
4400	1308.148	3371.816	2276.372	4819.954	499.918	4061.692	-48.217
4500	1309.093	3401.224	2301.043	4950.817	493.000	4142.786	-48.087
4600	1309.980	3430.007	2325.274	5081.771	485.588	4224.055	-47.965
4700	1310.812	3458.188	2349.080	5212.811	477.704	4305.340	-47.847
4800	1311.595	3485.794	2372.475	5343.932	469.406	4386.936	-47.739
4900	1312.333	3512.846	2395.472	5475.129	460.598	4468.531	-47.634
5000	1313.027	3539.365	2418.086	5606.397	451.404	4550.552	-47.538

3.648. Tetrabenzo[*a,f,k,n*]perylene



Formula: C₃₆H₂₀
Mass: 452.544 g/mol
CAS Number: 128746-59-8
Point Group: C₂

Length: 14.50 Å
Width: 13.98 Å
Breadth: 5.765 Å
L/B Ratio: 1.037

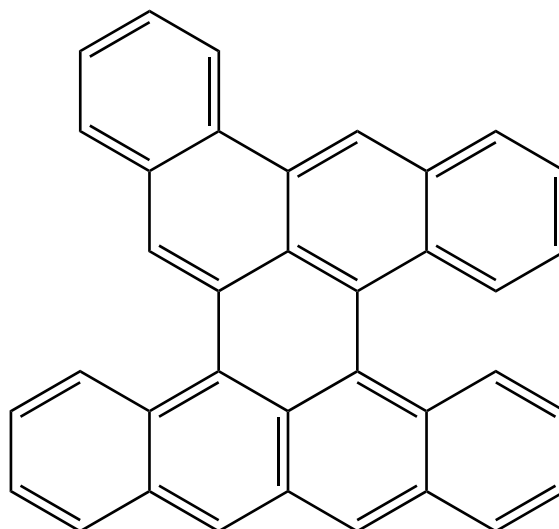
Cartesian coordinates:

C	-2.3396	-4.7907	0.3810	C	0.9292	-2.3868	-0.2315	H	-5.1840	-3.5095	-1.0003
C	-3.6463	-4.7561	-0.1905	C	0.9351	0.0118	0.0247	H	-0.5877	-3.7187	0.9123
C	-4.1688	-3.5719	-0.5916	C	0.2108	1.2532	-0.0143	H	-5.0662	-1.1001	-1.0554
C	-1.5781	-3.6686	0.4392	C	0.9040	2.4181	-0.2179	H	-5.0822	1.2964	-0.7481
C	-2.0393	-2.4011	-0.0625	C	2.3409	0.0154	0.0422	H	-5.2158	3.6284	-0.1222
C	-3.4102	-2.3544	-0.4732	C	3.0500	1.2406	-0.2406	H	-4.1791	5.6426	0.9123
C	-4.0210	-1.1407	-0.7245	C	2.3162	2.4360	-0.3587	H	-1.8326	5.5497	1.7137
C	-3.3223	0.0565	-0.4782	C	2.9686	3.6624	-0.6464	H	-0.4481	3.5520	1.3402
C	-4.0258	1.2753	-0.4526	C	4.3222	3.6958	-0.8552	H	0.4427	-3.3338	-0.5069
C	-2.0131	2.3989	0.3397	C	5.0614	2.4988	-0.7993	H	0.3786	3.3813	-0.3000
C	-3.4063	2.4191	0.0171	C	4.4428	1.3102	-0.5043	H	2.3718	4.5798	-0.7084
C	-4.1675	3.6262	0.1978	C	2.3276	-2.4312	0.0270	H	4.8326	4.6383	-1.0774
C	-3.6059	4.7218	0.7652	C	3.0264	-1.2368	0.2773	H	6.1375	2.5243	-1.0005
C	-2.2479	4.6763	1.2000	C	4.3429	-1.3445	0.7860	H	5.0468	0.3929	-0.4865
C	-1.4896	3.5700	0.9904	C	4.9575	-2.5664	0.9206	H	4.8809	-0.4355	1.0877
C	-1.2566	-1.2313	-0.1200	C	4.2877	-3.7464	0.5503	H	5.9753	-2.6293	1.3198
C	-1.9249	0.0251	-0.2078	C	2.9863	-3.6813	0.1191	H	4.8027	-4.7091	0.6288
C	-1.2506	1.2519	0.0522	H	-1.9691	-5.7392	0.7838	H	2.4366	-4.5940	-0.1383
C	0.2079	-1.2322	-0.0682	H	-4.2148	-5.6876	-0.2746				

Table 3.648: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,f,k,n*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.633	726.320	726.320	∞
100	145.909	387.099	967.875	-58.078	758.598	824.043	-430.427
200	290.762	530.514	713.318	-36.561	741.439	896.351	-234.098
250	373.903	604.263	684.097	-19.958	733.426	936.006	-195.564
298.15	454.899	677.063	677.063	0.000	726.320	975.686	-170.933
300	457.973	679.886	677.072	0.844	726.058	977.231	-170.147
350	538.799	756.615	682.947	25.784	719.552	1019.623	-152.167
400	613.742	833.529	696.965	54.625	713.951	1062.871	-138.794
450	681.607	909.807	716.386	87.040	709.147	1106.781	-128.469
500	742.236	984.822	739.491	122.665	705.025	1151.215	-120.264
600	843.786	1129.494	792.545	202.170	698.432	1241.110	-108.046
700	923.940	1265.821	850.521	290.710	693.764	1331.959	-99.390
800	988.094	1393.537	910.504	386.426	690.794	1423.337	-92.932
900	1040.278	1513.032	970.886	487.931	689.299	1514.990	-87.926
1000	1083.319	1624.934	1030.756	594.178	689.078	1606.755	-83.927
1100	1119.212	1729.919	1089.595	704.357	689.883	1698.505	-80.654
1200	1149.413	1828.635	1147.110	817.831	691.541	1790.118	-77.920
1300	1175.013	1921.676	1203.148	934.087	693.823	1881.581	-75.601
1400	1196.854	2009.574	1257.639	1052.708	696.564	1972.855	-73.607
1500	1215.598	2092.804	1310.568	1173.354	699.666	2063.923	-71.871
1600	1231.773	2171.786	1361.947	1295.743	702.964	2154.763	-70.344
1700	1245.802	2246.892	1411.811	1419.638	706.367	2245.363	-68.990
1800	1258.031	2318.454	1460.208	1544.843	709.781	2335.846	-67.783
1900	1268.740	2386.766	1507.190	1671.193	713.167	2426.071	-66.696
2000	1278.159	2452.088	1552.814	1798.548	716.458	2516.153	-65.714
2100	1286.480	2514.655	1597.137	1926.788	719.554	2606.057	-64.821
2200	1293.860	2574.676	1640.216	2055.813	722.457	2695.821	-64.006
2300	1300.431	2632.338	1682.106	2185.534	725.159	2785.458	-63.258
2400	1306.303	2687.810	1722.862	2315.876	727.572	2874.918	-62.570
2500	1311.569	2741.245	1762.535	2446.774	729.710	2964.432	-61.937
2600	1316.307	2792.780	1801.175	2578.172	731.528	3053.714	-61.349
2700	1320.583	2842.539	1838.828	2710.020	733.032	3143.028	-60.804
2800	1324.454	2890.637	1875.538	2842.275	734.189	3232.319	-60.298
2900	1327.968	2937.176	1911.348	2974.899	734.961	3321.507	-59.826
3000	1331.168	2982.251	1946.298	3107.858	735.406	3410.708	-59.384
3100	1334.088	3025.948	1980.424	3241.123	735.423	3499.799	-58.970
3200	1336.759	3068.346	2013.762	3374.667	735.067	3588.994	-58.583
3300	1339.210	3109.518	2046.346	3508.468	734.315	3678.257	-58.221
3400	1341.462	3149.532	2078.207	3642.503	733.131	3767.435	-57.878
3500	1343.536	3188.448	2109.375	3776.754	731.520	3856.629	-57.556
3600	1345.451	3226.323	2139.878	3911.205	729.513	3945.992	-57.254
3700	1347.222	3263.212	2169.742	4045.839	727.067	4035.437	-56.969
3800	1348.862	3299.162	2198.992	4180.645	724.150	4124.877	-56.699
3900	1350.385	3334.219	2227.653	4315.608	720.816	4214.329	-56.443
4000	1351.801	3368.426	2255.747	4450.718	717.042	4304.057	-56.204
4100	1353.119	3401.822	2283.294	4585.965	712.783	4393.787	-55.976
4200	1354.349	3434.444	2310.315	4721.339	708.075	4483.615	-55.761
4300	1355.498	3466.326	2336.830	4856.832	702.900	4573.442	-55.555
4400	1356.572	3497.501	2362.856	4992.436	697.270	4663.515	-55.362
4500	1357.579	3527.998	2388.410	5128.144	691.204	4753.795	-55.179
4600	1358.523	3557.847	2413.510	5263.950	684.634	4844.227	-55.007
4700	1359.410	3587.073	2438.169	5399.847	677.579	4934.656	-54.841
4800	1360.245	3615.702	2462.404	5535.830	670.100	5025.380	-54.686
4900	1361.030	3643.757	2486.228	5671.894	662.100	5116.086	-54.537
5000	1361.770	3671.261	2509.654	5808.034	653.702	5207.206	-54.398

3.649. Tetrabenzo[*a,e,j,o*]perylene



Formula: C₃₆H₂₀
Mass: 452.544 g/mol
CAS Number: 128721-01-7
Point Group: C₁

Length: 15.03 Å
Width: 13.47 Å
Breadth: 6.510 Å
L/B Ratio: 1.116

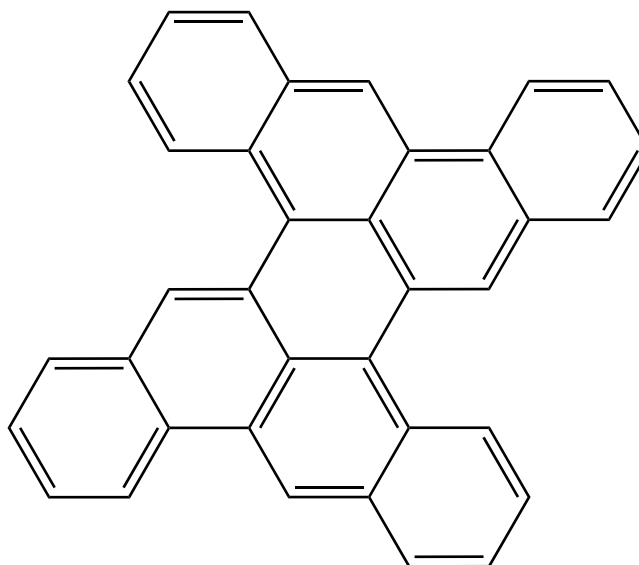
Cartesian coordinates:

C	2.5247	-4.1975	0.5333	C	-4.2878	2.8596	0.6693	H	-4.5929	3.8874	0.4423
C	2.1467	-2.8630	0.2945	C	-5.1257	2.0023	1.3045	H	-3.1420	-0.7818	1.4622
C	3.1373	-1.8811	0.1650	C	-4.6953	0.6768	1.6124	H	-2.3825	4.3762	-0.4804
C	4.4962	-2.2443	0.2560	C	-0.7137	2.9904	-0.4019	H	-0.0848	4.9647	-1.0508
C	4.8484	-3.5566	0.4923	C	-2.0645	3.3537	-0.2425	H	2.2210	5.6668	-1.2333
C	3.8574	-4.5377	0.6364	C	2.0098	2.4006	-0.0995	H	4.6053	5.3345	-0.5830
C	2.7586	-0.5124	-0.0398	C	1.5871	3.6939	-0.5513	H	5.2631	3.2678	0.6292
C	1.4634	-0.0837	0.0145	C	0.2447	3.9707	-0.7242	H	3.6755	1.4340	0.9469
C	0.4118	-1.0904	0.0500	C	2.5609	4.7307	-0.7756	H	0.0522	-4.5042	0.1482
C	0.7597	-2.4714	0.1317	C	3.8547	4.5562	-0.4134	H	3.5868	0.1809	-0.2447
C	1.0924	1.3316	-0.1028	C	4.2434	3.3474	0.2377	H	-2.2034	-5.1584	-0.5267
C	-0.2968	1.6470	-0.1810	C	3.3613	2.3271	0.3895	H	-4.4285	-4.5446	-1.4628
C	-1.2991	0.6666	0.0634	C	-1.5242	-3.0970	-0.3714	H	-4.9646	-2.1642	-1.9192
C	-0.9336	-0.7345	-0.1027	C	-0.2181	-3.4448	0.0090	H	-3.3797	-0.3748	-1.2989
C	-1.8738	-1.7317	-0.4967	C	-4.0082	-2.4127	-1.4473	H	5.2684	-1.4750	0.1414
C	-3.1318	-1.4255	-1.0995	C	-3.6931	-3.7744	-1.2091	H	5.9035	-3.8389	0.5690
C	-3.4716	0.2370	1.2205	C	-2.4777	-4.1101	-0.6900	H	4.1472	-5.5760	0.8275
C	-2.5633	1.0918	0.5058	H	-5.3705	0.0228	2.1739	H	1.7360	-4.9594	0.6273
C	-2.9616	2.4475	0.2983	H	-6.1330	2.3118	1.6008				

Table 3.649: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,e,j,o*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.551	735.966	735.966	∞
100	145.489	392.456	972.721	-58.026	768.295	833.204	-435.212
200	290.512	535.610	718.342	-36.546	751.099	904.992	-236.355
250	373.767	609.317	689.130	-19.953	743.076	944.393	-197.316
298.15	454.817	682.098	682.098	0.000	735.966	983.830	-172.359
300	457.892	684.921	682.107	0.844	735.704	985.366	-171.564
350	538.733	761.639	687.981	25.780	729.194	1027.507	-153.344
400	613.671	838.543	701.997	54.618	723.590	1070.504	-139.791
450	681.527	914.812	721.415	87.029	718.782	1114.163	-129.326
500	742.148	989.818	744.518	122.650	714.656	1158.348	-121.009
600	843.690	1134.474	797.565	202.145	708.053	1247.744	-108.623
700	923.844	1270.786	855.534	290.676	703.376	1338.095	-99.848
800	988.004	1398.489	915.511	386.383	700.396	1428.978	-93.301
900	1040.196	1517.974	975.886	487.879	698.893	1520.135	-88.225
1000	1083.243	1629.868	1035.750	594.118	698.664	1611.408	-84.170
1100	1119.144	1734.846	1094.582	704.290	699.462	1702.664	-80.851
1200	1149.351	1833.557	1152.092	817.757	701.113	1793.784	-78.080
1300	1174.957	1926.593	1208.125	934.007	703.389	1884.755	-75.729
1400	1196.803	2014.487	1262.613	1052.624	706.125	1975.538	-73.707
1500	1215.552	2097.713	1315.537	1173.265	709.222	2066.115	-71.947
1600	1231.731	2176.692	1366.912	1295.648	712.516	2156.465	-70.400
1700	1245.764	2251.796	1416.773	1419.540	715.915	2246.574	-69.027
1800	1257.996	2323.356	1465.167	1544.741	719.325	2336.567	-67.804
1900	1268.707	2391.666	1512.146	1671.088	722.708	2426.301	-66.702
2000	1278.130	2456.987	1557.767	1798.440	725.996	2515.894	-65.707
2100	1286.453	2519.552	1602.087	1926.677	729.089	2605.308	-64.802
2200	1293.835	2579.572	1645.163	2055.699	731.989	2694.582	-63.976
2300	1300.408	2637.233	1687.051	2185.417	734.689	2783.729	-63.219
2400	1306.281	2692.704	1727.805	2315.757	737.099	2872.700	-62.521
2500	1311.549	2746.138	1767.477	2446.654	739.235	2961.725	-61.881
2600	1316.288	2797.672	1806.114	2578.050	741.051	3050.517	-61.284
2700	1320.565	2847.430	1843.765	2709.896	742.553	3139.342	-60.733
2800	1324.437	2895.527	1880.474	2842.149	743.709	3228.145	-60.221
2900	1327.953	2942.066	1916.283	2974.771	744.479	3316.843	-59.742
3000	1331.153	2987.140	1951.231	3107.729	744.923	3405.555	-59.295
3100	1334.074	3030.837	1985.356	3240.993	744.938	3494.158	-58.875
3200	1336.746	3073.235	2018.693	3374.536	744.581	3582.863	-58.483
3300	1339.197	3114.407	2051.275	3508.335	743.828	3671.638	-58.116
3400	1341.450	3154.420	2083.135	3642.369	742.642	3760.326	-57.769
3500	1343.525	3193.336	2114.302	3776.619	741.030	3849.032	-57.442
3600	1345.440	3231.211	2144.803	3911.068	739.022	3937.906	-57.136
3700	1347.212	3268.099	2174.666	4045.702	736.576	4026.863	-56.848
3800	1348.853	3304.049	2203.916	4180.506	733.658	4115.814	-56.575
3900	1350.376	3339.106	2232.576	4315.469	730.322	4204.777	-56.316
4000	1351.792	3373.313	2260.668	4450.578	726.547	4294.017	-56.073
4100	1353.111	3406.708	2288.215	4585.824	722.287	4383.258	-55.842
4200	1354.341	3439.330	2315.235	4721.197	717.579	4472.597	-55.624
4300	1355.490	3471.212	2341.749	4856.689	712.403	4561.935	-55.415
4400	1356.565	3502.386	2367.774	4992.293	706.772	4651.520	-55.219
4500	1357.572	3532.884	2393.328	5128.000	700.706	4741.311	-55.035
4600	1358.517	3562.732	2418.427	5263.805	694.135	4831.255	-54.859
4700	1359.404	3591.958	2443.086	5399.701	687.079	4921.195	-54.692
4800	1360.239	3620.587	2467.320	5535.684	679.600	5011.431	-54.534
4900	1361.024	3648.643	2491.143	5671.748	671.599	5101.648	-54.383
5000	1361.765	3676.146	2514.569	5807.887	663.201	5192.279	-54.242

3.650. Dinaphtho[3,2,1-*fg*:3',2',1'-*qr*]pentacene



Formula: $C_{36}H_{20}$
Mass: 452.544 g/mol
CAS Number: 128721-00-6
Point Group: C_2

Length: 15.85 Å
Width: 13.64 Å
Breadth: 6.654 Å
L/B Ratio: 1.162

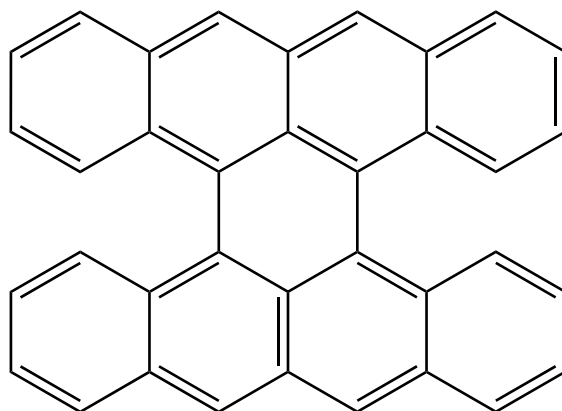
Cartesian coordinates:

C	2.0582	4.5875	0.9960	C	-1.7926	-3.2437	0.5977	H	-3.8832	-2.8041	0.1801
C	1.7929	3.2449	0.5897	C	-0.4602	-2.7613	0.5594	H	-1.9981	2.7438	-0.7221
C	0.4607	2.7616	0.5547	C	-3.7280	-0.2068	-0.4742	H	-5.2415	-1.7463	-0.3615
C	-0.5688	3.6511	0.9886	C	-3.4613	1.1381	-0.7728	H	-7.0735	-0.2472	-1.1510
C	-0.2898	4.9234	1.3951	C	-2.1396	1.6635	-0.5693	H	-6.5892	2.1222	-1.7185
C	1.0422	5.4074	1.3880	C	-5.0421	-0.6922	-0.6083	H	-4.2847	3.0190	-1.4688
C	0.2228	1.4186	0.1446	C	-6.0537	0.1371	-1.0465	H	1.6090	-3.2954	0.9981
C	1.3094	0.5523	-0.0178	C	-5.7808	1.4745	-1.3638	H	1.0934	-5.5859	1.7391
C	2.6343	1.0711	-0.0722	C	-4.5014	1.9722	-1.2271	H	-1.2388	-6.4358	1.7119
C	2.8569	2.4058	0.2181	C	0.5694	-3.6515	0.9921	H	-3.0960	-4.9383	1.0032
C	1.1090	-0.8804	-0.1498	C	0.2903	-4.9235	1.3992	H	5.2406	1.7477	-0.3751
C	-0.2222	-1.4188	0.1474	C	-1.0419	-5.4069	1.3943	H	7.0721	0.2472	-1.1629
C	-1.3091	-0.5525	-0.0146	C	-2.0580	-4.5861	1.0045	H	6.5880	-2.1241	-1.7229
C	-1.1087	0.8799	-0.1502	C	5.0413	0.6928	-0.6185	H	4.2843	-3.0212	-1.4673
C	3.7276	0.2071	-0.4809	C	6.0526	-0.1373	-1.0558	H	-1.6083	3.2947	0.9967
C	3.4611	-1.1388	-0.7752	C	5.7799	-1.4758	-1.3688	H	-1.0927	5.5857	1.7358
C	2.1401	-1.6645	-0.5677	C	4.5010	-1.9737	-1.2287	H	1.2390	6.4363	1.7059
C	-2.6343	-1.0705	-0.0656	H	3.8826	2.8060	0.1667	H	3.0959	4.9405	0.9924
C	-2.8571	-2.4045	0.2276	H	1.9996	-2.7455	-0.7164				

Table 3.650: Table of thermodynamic data as a function of temperature for Dinaphtho[3,2,1-*fg*:3',2',1'-*qr*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.762	653.626	653.626	∞
100	147.172	391.257	971.824	-58.057	685.925	750.954	-392.250
200	290.535	535.060	717.523	-36.493	668.813	822.816	-214.893
250	373.174	608.701	688.361	-19.915	660.775	862.246	-180.153
298.15	453.841	681.342	681.342	0.000	653.626	901.716	-157.974
300	456.905	684.159	681.351	0.842	653.362	903.253	-157.267
350	537.525	760.706	687.212	25.723	646.797	945.436	-141.096
400	612.362	837.442	701.198	54.498	641.130	988.484	-129.080
450	680.195	913.555	720.573	86.842	636.256	1032.202	-119.812
500	740.840	988.422	743.627	122.397	632.063	1076.453	-112.454
600	842.502	1132.849	796.570	201.767	625.335	1166.001	-101.507
700	922.809	1268.989	854.437	290.186	620.546	1256.524	-93.761
800	987.117	1396.564	914.317	385.797	617.471	1347.593	-87.987
900	1039.439	1515.952	974.606	487.212	615.885	1438.948	-83.513
1000	1082.597	1627.772	1034.392	593.380	615.586	1530.426	-79.940
1100	1118.590	1732.693	1093.154	703.493	616.325	1621.895	-77.016
1200	1148.874	1831.359	1150.602	816.909	617.924	1713.233	-74.574
1300	1174.543	1924.359	1206.579	933.114	620.156	1804.426	-72.501
1400	1196.441	2012.224	1261.016	1051.692	622.853	1895.433	-70.718
1500	1215.234	2095.427	1313.895	1172.299	625.917	1986.238	-69.166
1600	1231.450	2174.387	1365.229	1294.653	629.180	2076.817	-67.800
1700	1245.514	2249.475	1415.053	1418.517	632.553	2167.158	-66.587
1800	1257.772	2321.022	1463.413	1543.695	635.939	2257.383	-65.506
1900	1268.506	2389.320	1510.361	1670.021	639.301	2347.352	-64.532
2000	1277.947	2454.631	1555.954	1797.353	642.569	2437.180	-63.651
2100	1286.287	2517.188	1600.248	1925.574	645.645	2526.830	-62.850
2200	1293.684	2577.200	1643.300	2054.579	648.529	2616.341	-62.119
2300	1300.270	2634.855	1685.166	2184.283	651.215	2705.725	-61.448
2400	1306.155	2690.320	1725.900	2314.610	653.612	2794.934	-60.829
2500	1311.432	2743.749	1765.551	2445.494	655.736	2884.198	-60.261
2600	1316.180	2795.279	1804.171	2576.879	657.541	2973.229	-59.732
2700	1320.465	2845.033	1841.806	2708.715	659.033	3062.293	-59.242
2800	1324.344	2893.127	1878.499	2840.958	660.178	3151.336	-58.788
2900	1327.866	2939.662	1914.293	2973.572	660.939	3240.274	-58.362
3000	1331.072	2984.734	1949.227	3106.521	661.375	3329.227	-57.966
3100	1333.998	3028.428	1983.339	3239.777	661.383	3418.070	-57.593
3200	1336.675	3070.823	2016.663	3373.312	661.018	3507.017	-57.245
3300	1339.130	3111.993	2049.234	3507.104	660.258	3596.033	-56.919
3400	1341.387	3152.004	2081.083	3641.132	659.066	3684.963	-56.611
3500	1343.466	3190.918	2112.239	3775.376	657.448	3773.910	-56.321
3600	1345.384	3228.792	2142.731	3909.820	655.433	3863.026	-56.050
3700	1347.158	3265.679	2172.585	4044.448	652.982	3952.225	-55.794
3800	1348.802	3301.627	2201.825	4179.247	650.059	4041.418	-55.552
3900	1350.328	3336.683	2230.477	4314.204	646.718	4130.624	-55.322
4000	1351.747	3370.888	2258.561	4449.309	642.939	4220.105	-55.108
4100	1353.068	3404.283	2286.100	4584.551	638.674	4309.589	-54.904
4200	1354.300	3436.904	2313.113	4719.920	633.961	4399.171	-54.711
4300	1355.451	3468.785	2339.620	4855.408	628.782	4488.752	-54.526
4400	1356.528	3499.958	2365.638	4991.007	623.147	4578.579	-54.354
4500	1357.536	3530.455	2391.185	5126.711	617.077	4668.613	-54.191
4600	1358.483	3560.302	2416.278	5262.513	610.502	4758.800	-54.037
4700	1359.371	3589.528	2440.931	5398.406	603.444	4848.983	-53.889
4800	1360.207	3618.156	2465.159	5534.385	595.961	4939.462	-53.751
4900	1360.994	3646.211	2488.977	5670.445	587.957	5029.922	-53.619
5000	1361.736	3673.714	2512.397	5806.582	579.556	5120.797	-53.495

3.651. Tetrabenzo[*a,f,j,o*]perylene



Formula: C₃₆H₂₀
Mass: 452.544 g/mol
CAS Number: 191-03-7
Point Group: D₂

Length: 13.11 Å
Width: 11.63 Å
Breadth: 7.628 Å
L/B Ratio: 1.127

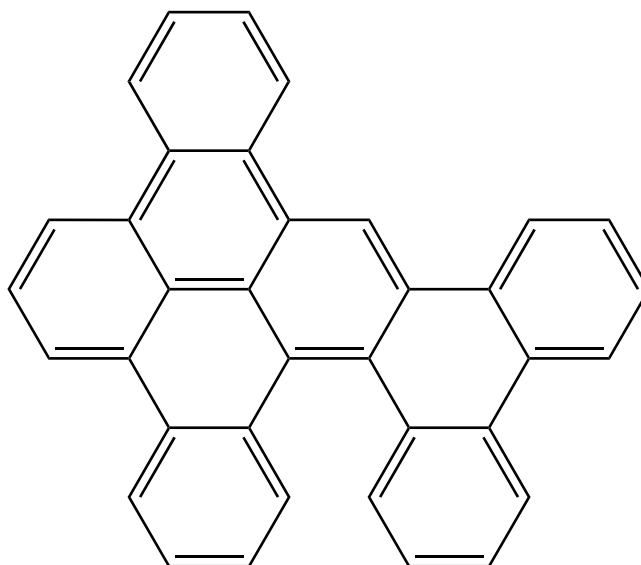
Cartesian coordinates:

C	-3.4021	-3.5137	-1.3946	C	-0.0002	-1.4081	0.0008	H	-3.3671	4.6098	1.4227
C	-2.2695	-2.8144	-0.8497	C	-0.0001	-2.8294	0.0011	H	-3.4699	0.3833	-1.2762
C	-2.3113	-1.3876	-0.7507	C	-1.1574	-3.5175	-0.4132	H	-1.1600	4.6147	0.4101
C	-3.4592	-0.7145	-1.2930	C	2.3111	1.3861	-0.7534	H	1.1631	4.6136	-0.4135
C	-4.4933	-1.4070	-1.8356	C	2.2702	2.8129	-0.8524	H	3.3696	4.6063	-1.4279
C	-4.4759	-2.8339	-1.8683	C	1.1587	3.5166	-0.4157	H	5.3380	3.3572	-2.2942
C	-1.2218	-0.7053	-0.1909	C	2.3106	-1.3868	0.7530	H	5.3520	0.8787	-2.2689
C	-1.2215	0.7056	0.1912	C	3.4575	-0.7128	1.2961	H	3.4676	0.3850	1.2784
C	-2.3105	1.3882	0.7513	C	3.4579	0.7119	-1.2965	H	-1.1608	-4.6144	-0.4121
C	-3.4578	0.7153	1.2952	C	4.4918	1.4035	-1.8406	H	1.1613	-4.6139	0.4142
C	-2.2689	2.8151	0.8489	C	4.4760	2.8305	-1.8724	H	3.4677	-0.3859	-1.2789
C	-3.4018	3.5147	1.3927	C	3.4034	3.5112	-1.3973	H	5.3515	-0.8799	2.2689
C	-4.4753	2.8352	1.8674	C	1.1575	-3.5170	0.4158	H	5.3365	-3.3584	2.2952
C	-4.4920	1.4082	1.8373	C	2.2691	-2.8135	0.8527	H	3.3674	-4.6071	1.4298
C	-1.1567	3.5178	0.4121	C	3.4018	-3.5121	1.3984	H	-3.3666	-4.6086	-1.4269
C	0.0007	2.8293	-0.0016	C	4.4747	-2.8315	1.8730	H	-5.3375	-3.3614	-2.2901
C	0.0002	1.4080	-0.0012	C	4.4912	-1.4046	1.8405	H	-5.3550	-0.8828	-2.2618
C	1.2216	0.7048	-0.1926	H	-5.3529	0.8843	2.2655	H	-3.4679	-0.3825	1.2801
C	1.2214	-0.7053	0.1919	H	-5.3373	3.3630	2.2879				

Table 3.651: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,f,j,o*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.786	749.224	749.224	∞
100	145.682	376.519	959.971	-58.345	781.235	847.738	-442.804
200	292.285	520.354	704.142	-36.758	764.147	921.091	-240.559
250	375.956	594.505	674.764	-20.065	756.224	961.244	-200.837
298.15	457.226	667.693	667.693	0.000	749.224	1001.384	-175.435
300	460.307	670.530	667.701	0.849	748.967	1002.946	-174.625
350	541.231	747.628	673.605	25.908	742.580	1045.797	-156.073
400	616.152	824.866	687.689	54.871	737.101	1089.486	-142.269
450	683.929	901.424	707.193	87.404	732.416	1133.822	-131.608
500	744.436	976.677	730.392	123.142	728.407	1178.669	-123.132
600	845.715	1121.726	783.638	202.853	722.020	1269.359	-110.505
700	925.617	1258.331	841.797	291.573	717.532	1360.970	-101.555
800	989.557	1386.256	901.948	387.446	714.719	1453.086	-94.875
900	1041.563	1505.913	962.482	489.088	713.361	1545.458	-89.694
1000	1084.454	1617.943	1022.487	595.456	713.260	1637.929	-85.555
1100	1120.222	1723.030	1081.446	705.742	714.173	1730.372	-82.167
1200	1150.316	1821.829	1139.070	819.312	715.926	1822.670	-79.337
1300	1175.824	1914.939	1195.206	935.653	718.294	1914.810	-76.936
1400	1197.586	2002.894	1249.785	1054.352	721.112	2006.755	-74.871
1500	1216.261	2086.172	1302.793	1175.068	724.284	2098.488	-73.074
1600	1232.375	2165.194	1354.245	1297.519	727.645	2189.990	-71.494
1700	1246.352	2240.336	1404.176	1421.471	731.106	2281.248	-70.093
1800	1258.534	2311.928	1452.634	1546.729	734.572	2372.384	-68.843
1900	1269.201	2380.266	1499.672	1673.128	738.006	2463.260	-67.718
2000	1278.584	2445.611	1545.347	1800.527	741.341	2553.992	-66.702
2100	1286.872	2508.198	1589.718	1928.808	744.479	2644.542	-65.778
2200	1294.223	2568.236	1632.841	2057.870	747.419	2734.951	-64.935
2300	1300.767	2625.914	1674.772	2187.626	750.156	2825.231	-64.162
2400	1306.616	2681.400	1715.566	2318.000	752.601	2915.333	-63.449
2500	1311.860	2734.847	1755.275	2448.929	754.769	3005.488	-62.795
2600	1316.579	2786.392	1793.948	2580.355	756.615	3095.408	-62.186
2700	1320.837	2836.162	1831.632	2712.229	758.146	3185.361	-61.623
2800	1324.692	2884.268	1868.372	2844.509	759.327	3275.290	-61.100
2900	1328.192	2930.815	1904.210	2977.156	760.122	3365.113	-60.611
3000	1331.378	2975.898	1939.185	3110.137	760.589	3454.950	-60.155
3100	1334.286	3019.601	1973.336	3243.422	760.627	3544.677	-59.726
3200	1336.947	3062.006	2006.698	3376.986	760.290	3634.505	-59.326
3300	1339.386	3103.184	2039.304	3510.804	759.557	3724.403	-58.951
3400	1341.629	3143.202	2071.186	3644.857	758.389	3814.213	-58.597
3500	1343.695	3182.123	2102.373	3779.124	756.795	3904.040	-58.263
3600	1345.601	3220.003	2132.895	3913.590	754.803	3994.035	-57.951
3700	1347.365	3256.896	2162.777	4048.240	752.372	4084.113	-57.656
3800	1348.998	3292.849	2192.044	4183.059	749.469	4174.184	-57.377
3900	1350.514	3327.910	2220.722	4318.035	746.148	4264.267	-57.112
4000	1351.924	3362.120	2248.831	4453.158	742.387	4354.626	-56.864
4100	1353.237	3395.519	2276.393	4588.417	738.139	4444.986	-56.629
4200	1354.461	3428.144	2303.429	4723.803	733.443	4535.444	-56.405
4300	1355.605	3460.028	2329.957	4859.307	728.279	4625.901	-56.192
4400	1356.675	3491.205	2355.996	4994.921	722.660	4716.604	-55.992
4500	1357.678	3521.705	2381.563	5130.639	716.604	4807.513	-55.803
4600	1358.618	3551.556	2406.674	5266.455	710.043	4898.574	-55.624
4700	1359.501	3580.784	2431.346	5402.361	702.998	4989.632	-55.452
4800	1360.332	3609.415	2455.591	5538.353	695.528	5080.985	-55.291
4900	1361.114	3637.472	2479.426	5674.426	687.536	5172.319	-55.136
5000	1361.851	3664.978	2502.863	5810.574	679.147	5264.068	-54.992

3.652. Dibenzo[*f,j*]naphtho[1,2,3,4-*pqr*]picene



Formula: C₃₆H₂₀
Mass: 452.544 g/mol
CAS Number: 133156-50-0
Point Group: C₁

Length: 15.65 Å
Width: 13.88 Å
Breadth: 6.872 Å
L/B Ratio: 1.127

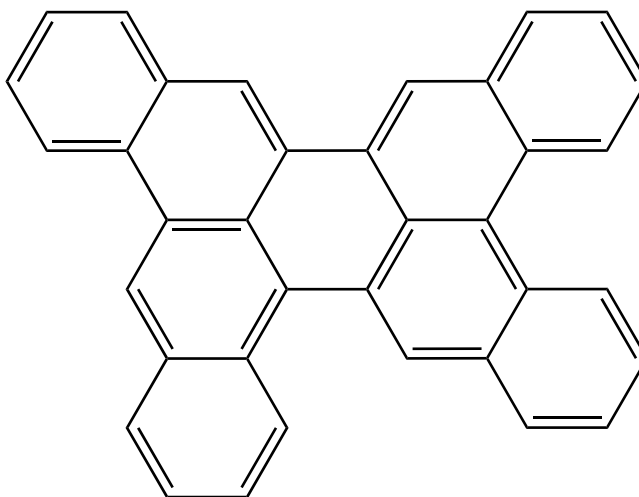
Cartesian coordinates:

C	2.6948	3.2705	0.6722	C	-3.8183	-2.6394	-0.2356	H	-5.9079	-2.3688	-0.6834
C	2.6006	1.9234	0.2797	C	-4.9485	-1.8776	-0.4907	H	-3.8784	-3.7379	-0.1999
C	3.7780	1.1854	0.0834	C	-4.8685	-0.4911	-0.4867	H	-2.5145	-4.6481	0.5466
C	5.0226	1.7937	0.3216	C	-0.1674	-2.1612	0.5120	H	-0.5819	-5.9207	1.4809
C	5.0963	3.1110	0.7296	C	-1.4150	-2.7958	0.3797	H	1.5680	-4.7460	1.9270
C	3.9251	3.8565	0.8969	C	2.3533	-2.0131	-1.2476	H	1.3706	-2.4697	-1.4236
C	3.6863	-0.1724	-0.4265	C	0.8863	-2.8776	1.1112	H	-1.2864	4.1193	0.1600
C	2.4307	-0.7955	-0.5448	C	0.7367	-4.2049	1.4633	H	-3.3505	5.4924	-0.0779
C	1.2311	-0.1189	-0.0636	C	-0.4755	-4.8607	1.2291	H	-5.5492	4.3821	-0.4302
C	1.3060	1.2756	0.1274	C	-1.5412	-4.1583	0.7042	H	-5.6888	1.8981	-0.5251
C	-0.0205	-0.7558	0.1482	C	-2.2646	3.6371	0.0095	H	1.8403	-2.3692	1.3024
C	-1.1957	0.0198	0.0731	C	-3.4088	4.4002	-0.1240	H	3.4105	-3.5852	-2.2637
C	-1.1146	1.4323	0.0693	C	-4.6438	3.7766	-0.3198	H	5.6492	-2.5722	-1.8617
C	0.1309	2.0322	0.1974	C	-4.7199	2.3979	-0.3724	H	5.8171	-0.3525	-0.7355
C	-2.4859	-0.6172	-0.0477	C	3.4908	-2.6374	-1.7213	H	5.9369	1.2012	0.1641
C	-3.6496	0.1536	-0.2596	C	4.7469	-2.0616	-1.5104	H	6.0697	3.5757	0.9168
C	-3.5670	1.6070	-0.2309	C	4.8392	-0.8373	-0.8799	H	3.9863	4.9042	1.2084
C	-2.3243	2.2340	-0.0453	H	0.1995	3.1298	0.3208	H	1.7679	3.8501	0.8015
C	-2.5859	-2.0223	0.0020	H	-5.7693	0.1170	-0.6619				

Table 3.652: Table of thermodynamic data as a function of temperature for Dibenzof[*f,j*]naphtho[1,2,3,4-*pqr*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.720	623.655	623.655	∞
100	147.471	399.112	978.489	-57.938	656.073	720.316	-376.247
200	289.866	542.799	724.778	-36.396	638.939	791.394	-206.687
250	372.154	616.252	695.694	-19.861	630.858	830.441	-173.508
298.15	452.640	688.695	688.695	0.000	623.655	869.553	-152.339
300	455.701	691.504	688.704	0.840	623.389	871.076	-151.665
350	536.284	767.862	694.550	25.659	616.762	912.897	-136.240
400	611.171	844.434	708.502	54.373	611.034	955.591	-124.785
450	679.090	920.412	727.835	86.659	606.102	998.963	-115.954
500	739.827	995.167	750.843	122.162	601.857	1042.874	-108.946
600	841.640	1139.423	803.692	201.438	595.035	1131.756	-98.526
700	922.042	1275.438	861.471	289.777	590.166	1221.629	-91.157
800	986.405	1402.914	921.272	385.314	587.017	1312.058	-85.667
900	1038.762	1522.221	981.489	486.659	585.362	1402.782	-81.414
1000	1081.949	1633.971	1041.210	592.761	584.996	1493.637	-78.018
1100	1117.969	1738.832	1099.913	702.810	585.671	1584.489	-75.240
1200	1148.281	1837.445	1157.307	816.165	587.210	1675.216	-72.919
1300	1173.980	1930.399	1213.235	932.313	589.384	1765.803	-70.949
1400	1195.909	2018.223	1267.626	1050.836	592.027	1856.208	-69.255
1500	1214.732	2101.391	1320.463	1171.391	595.038	1946.414	-67.779
1600	1230.977	2180.319	1371.759	1293.696	598.253	2036.399	-66.480
1700	1245.070	2255.379	1421.547	1417.515	601.580	2126.148	-65.327
1800	1257.356	2326.901	1469.873	1542.650	604.923	2215.784	-64.299
1900	1268.116	2395.177	1516.790	1668.935	608.244	2305.166	-63.372
2000	1277.582	2460.469	1562.354	1796.230	611.475	2394.409	-62.534
2100	1285.944	2523.009	1606.621	1924.415	614.516	2483.476	-61.772
2200	1293.362	2583.006	1649.648	2053.388	617.367	2572.406	-61.075
2300	1299.967	2640.646	1691.490	2183.060	620.021	2661.211	-60.437
2400	1305.871	2696.100	1732.200	2313.358	622.389	2749.841	-59.847
2500	1311.165	2749.517	1771.831	2444.214	624.485	2838.528	-59.307
2600	1315.928	2801.036	1810.431	2575.573	626.264	2926.982	-58.803
2700	1320.228	2850.782	1848.047	2707.384	627.731	3015.471	-58.337
2800	1324.120	2898.867	1884.722	2839.605	628.854	3103.939	-57.904
2900	1327.654	2945.395	1920.499	2972.197	629.593	3192.304	-57.498
3000	1330.872	2990.459	1955.417	3105.125	630.008	3280.684	-57.121
3100	1333.809	3034.147	1989.514	3238.362	629.997	3368.955	-56.765
3200	1336.496	3076.537	2022.825	3371.879	629.614	3457.330	-56.434
3300	1338.960	3117.701	2055.382	3505.653	628.836	3545.775	-56.124
3400	1341.225	3157.707	2087.218	3639.664	627.627	3634.134	-55.831
3500	1343.312	3196.616	2118.362	3773.892	625.993	3722.512	-55.554
3600	1345.237	3234.486	2148.841	3908.321	623.964	3811.058	-55.296
3700	1347.019	3271.369	2178.684	4042.935	621.498	3899.688	-55.053
3800	1348.669	3307.314	2207.914	4177.720	618.561	3988.312	-54.822
3900	1350.201	3342.366	2236.555	4312.665	615.208	4076.949	-54.603
4000	1351.625	3376.568	2264.629	4447.757	611.416	4165.863	-54.399
4100	1352.951	3409.960	2292.158	4582.987	607.139	4254.779	-54.205
4200	1354.188	3442.578	2319.162	4718.344	602.415	4343.793	-54.022
4300	1355.344	3474.456	2345.660	4853.822	597.224	4432.806	-53.847
4400	1356.425	3505.627	2371.670	4989.411	591.580	4522.067	-53.683
4500	1357.438	3536.122	2397.210	5125.104	585.499	4611.534	-53.528
4600	1358.388	3565.967	2422.294	5260.896	578.915	4701.154	-53.382
4700	1359.281	3595.191	2446.940	5396.780	571.847	4790.771	-53.242
4800	1360.120	3623.817	2471.161	5532.751	564.355	4880.684	-53.112
4900	1360.910	3651.870	2494.971	5668.802	556.343	4970.578	-52.986
5000	1361.655	3679.372	2518.385	5804.931	547.934	5060.886	-52.870

3.653. Dinaphtho[1,2,3-*fg*:3',2',1'-*qr*]pentacene



Formula: $C_{36}H_{20}$
Mass: 452.544 g/mol
CAS Number: 128720-98-9
Point Group: C_1

Length: 15.69 Å
Width: 12.86 Å
Breadth: 5.374 Å
L/B Ratio: 1.220

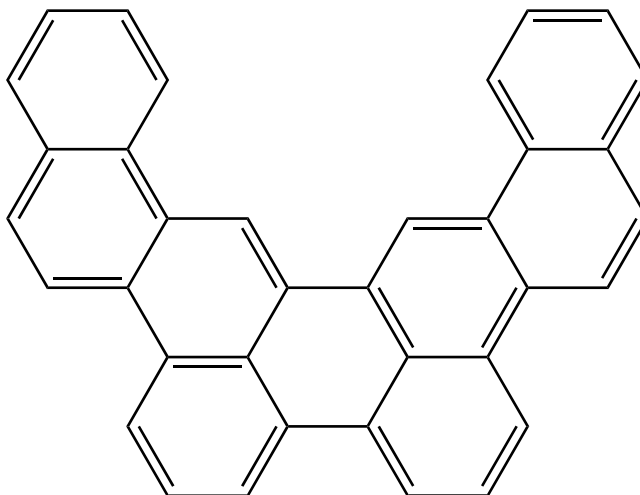
Cartesian coordinates:

C	-5.3742	3.5339	-0.4242	C	-3.7443	-1.2905	-0.0109	H	-5.8119	0.1483	-0.3220
C	-6.0295	2.2951	-0.4344	C	-1.5789	-2.4029	0.2328	H	-3.4842	4.5557	-0.2854
C	-5.3066	1.1262	-0.3173	C	-2.9948	-2.4612	0.1872	H	-1.3424	3.4384	0.0393
C	-4.0021	3.5900	-0.2953	C	-3.6710	-3.7066	0.3640	H	0.7924	-3.0100	-1.0025
C	-3.2527	2.4033	-0.1765	C	-2.9717	-4.8433	0.6395	H	2.8990	-4.0686	-1.3708
C	-3.9050	1.1607	-0.1896	C	-1.5610	-4.7858	0.7613	H	5.3476	-4.1741	-0.9281
C	-1.8260	2.4503	-0.0304	C	-0.8935	-3.6128	0.5616	H	6.4739	-2.2624	0.1942
C	-1.0735	1.3174	0.0422	C	0.3776	1.4007	0.2035	H	5.2434	-0.1957	0.6866
C	0.5223	-1.0327	-0.1972	C	1.1850	0.2287	0.0269	H	-4.8422	-1.3470	-0.0908
C	1.2703	-2.0792	-0.6637	C	2.5853	0.3271	0.0139	H	-4.7641	-3.7245	0.2845
C	3.3521	-0.8910	-0.1429	C	0.9691	2.6025	0.4826	H	-3.4830	-5.8009	0.7800
C	2.6928	-2.0422	-0.6177	C	2.3821	2.7439	0.4460	H	-1.0142	-5.6975	1.0241
C	3.4265	-3.2113	-0.9367	C	3.1923	1.6362	0.1206	H	0.2001	-3.5936	0.6654
C	4.7732	-3.2749	-0.6834	C	4.5597	1.9036	-0.1461	H	0.3472	3.4934	0.6685
C	5.4150	-2.1821	-0.0732	C	5.0974	3.1553	0.0210	H	5.2108	1.0986	-0.5124
C	4.7220	-1.0258	0.1910	C	4.2952	4.2260	0.4577	H	6.1572	3.3318	-0.1911
C	-0.9269	-1.1542	0.0081	C	2.9535	4.0250	0.6517	H	4.7446	5.2111	0.6178
C	-1.6989	0.0133	-0.0162	H	-5.9577	4.4555	-0.5187	H	2.3029	4.8533	0.9552
C	-3.1207	-0.0565	-0.0690	H	-7.1191	2.2600	-0.5359				

Table 3.653: Table of thermodynamic data as a function of temperature for Dinaphtho[1,2,3-*fg*:3',2',1'-*qr*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.621	655.773	655.773	∞
100	146.500	397.783	977.264	-57.948	688.181	752.557	-393.087
200	289.954	541.147	723.382	-36.447	671.006	823.791	-215.148
250	372.705	614.671	694.253	-19.895	662.942	862.920	-180.294
298.15	453.509	687.241	687.241	0.000	655.773	902.104	-158.042
300	456.578	690.055	687.249	0.842	655.509	903.631	-157.333
350	537.335	766.563	693.107	25.710	648.931	945.520	-141.108
400	612.285	843.281	707.086	54.478	643.257	988.276	-129.053
450	680.200	919.390	726.456	86.820	638.381	1031.702	-119.754
500	740.902	994.260	749.505	122.377	634.190	1075.661	-112.371
600	842.620	1138.704	802.443	201.757	627.472	1164.624	-101.387
700	922.935	1274.863	860.308	290.188	622.696	1254.561	-93.615
800	987.231	1402.454	920.190	385.811	619.632	1345.042	-87.820
900	1039.534	1521.855	980.482	487.236	618.057	1435.807	-83.330
1000	1082.673	1633.684	1040.271	593.414	617.767	1526.694	-79.745
1100	1118.648	1738.612	1099.037	703.533	618.512	1617.572	-76.810
1200	1148.917	1837.282	1156.487	816.953	620.117	1708.318	-74.360
1300	1174.575	1930.285	1212.467	933.163	622.352	1798.918	-72.280
1400	1196.464	2018.152	1266.907	1051.743	625.052	1889.333	-70.490
1500	1215.250	2101.357	1319.789	1172.352	628.117	1979.544	-68.932
1600	1231.460	2180.317	1371.125	1294.707	631.382	2069.531	-67.562
1700	1245.520	2255.406	1420.951	1418.573	634.756	2159.279	-66.345
1800	1257.775	2326.952	1469.313	1543.751	638.142	2248.911	-65.260
1900	1268.506	2395.251	1516.263	1670.077	641.504	2338.286	-64.283
2000	1277.946	2460.562	1561.857	1797.409	644.772	2427.521	-63.399
2100	1286.285	2523.119	1606.152	1925.629	647.848	2516.578	-62.595
2200	1293.680	2583.131	1649.206	2054.635	650.732	2605.496	-61.861
2300	1300.265	2640.785	1691.073	2184.338	653.417	2694.288	-61.188
2400	1306.150	2696.251	1731.807	2314.664	655.814	2782.903	-60.567
2500	1311.426	2749.679	1771.460	2445.548	657.937	2871.574	-59.997
2600	1316.174	2801.208	1810.081	2576.932	659.741	2960.012	-59.466
2700	1320.459	2850.963	1847.716	2708.767	661.232	3048.484	-58.975
2800	1324.338	2899.056	1884.410	2841.010	662.377	3136.933	-58.519
2900	1327.860	2945.591	1920.204	2973.623	663.138	3225.279	-58.092
3000	1331.066	2990.663	1955.139	3106.572	663.573	3313.639	-57.694
3100	1333.992	3034.357	1989.251	3239.827	663.580	3401.889	-57.320
3200	1336.670	3076.752	2022.576	3373.362	663.215	3490.243	-56.971
3300	1339.125	3117.922	2055.148	3507.154	662.455	3578.666	-56.644
3400	1341.382	3157.932	2086.997	3641.180	661.262	3667.003	-56.335
3500	1343.460	3196.846	2118.154	3775.424	659.643	3755.357	-56.044
3600	1345.379	3234.720	2148.646	3909.867	657.628	3843.881	-55.772
3700	1347.153	3271.606	2178.500	4044.495	655.176	3932.486	-55.516
3800	1348.797	3307.555	2207.741	4179.294	652.253	4021.087	-55.273
3900	1350.323	3342.610	2236.392	4314.251	648.912	4109.700	-55.042
4000	1351.742	3376.816	2264.477	4449.355	645.132	4198.589	-54.827
4100	1353.063	3410.210	2292.016	4584.596	640.867	4287.480	-54.622
4200	1354.296	3442.831	2319.030	4719.964	636.153	4376.469	-54.428
4300	1355.447	3474.712	2345.537	4855.452	630.973	4465.457	-54.243
4400	1356.524	3505.885	2371.555	4991.051	625.338	4554.692	-54.070
4500	1357.532	3536.381	2397.103	5126.755	619.268	4644.133	-53.907
4600	1358.479	3566.229	2422.195	5262.556	612.693	4733.727	-53.752
4700	1359.368	3595.454	2446.848	5398.448	605.633	4823.318	-53.604
4800	1360.203	3624.083	2471.077	5534.427	598.150	4913.204	-53.465
4900	1360.990	3652.137	2494.895	5670.487	590.147	5003.071	-53.332
5000	1361.732	3679.640	2518.316	5806.624	581.745	5093.353	-53.209

3.654. Dinaphtho[1,2-*b*,2',1'-*n*]perylene



Formula: $C_{36}H_{20}$
Mass: 452.544 g/mol
CAS Number: 197-67-1
Point Group: C_{2v}

Length: 15.97 Å
Width: 12.87 Å
Breadth: 3.886 Å
L/B Ratio: 1.241

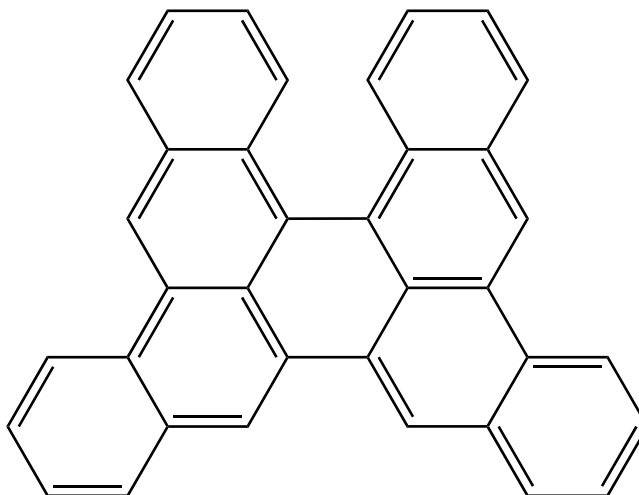
Cartesian coordinates:

C	0.7306	0.6142	0.0000	C	-5.6773	-0.5870	0.0000	H	3.3735	5.2468	0.0000
C	1.4356	-0.5602	0.0000	C	-3.5704	-1.8408	0.0000	H	0.8886	5.2448	0.0000
C	0.7284	3.0992	0.0000	C	-4.9773	-1.8339	0.0000	H	-0.8959	-1.5304	0.0000
C	1.4344	1.8653	0.0000	C	-5.6839	-3.0602	0.0000	H	-0.8991	5.2430	0.0000
C	2.8442	1.8692	0.0000	C	-5.0031	-4.2527	0.0000	H	-3.3840	5.2400	0.0000
C	3.5304	3.1059	0.0000	C	-3.5949	-4.2639	0.0000	H	-4.6371	3.0884	0.0000
C	2.8378	4.2918	0.0000	C	-2.8932	-3.0838	0.0000	H	-5.5295	1.5511	0.0000
C	1.4356	4.2894	0.0000	C	3.5651	0.6219	0.0000	H	-6.7732	-0.6017	0.0000
C	-0.7318	0.6128	0.0000	C	2.8589	-0.5821	0.0000	H	-6.7797	-3.0428	0.0000
C	-1.4345	-0.5631	0.0000	C	5.6784	-0.5757	0.0000	H	-5.5474	-5.2026	0.0000
C	-1.4381	1.8624	0.0000	C	4.9949	0.5981	0.0000	H	-3.0656	-5.2223	0.0000
C	-0.7346	3.0977	0.0000	C	4.9809	-1.8240	0.0000	H	-1.7925	-3.0798	0.0000
C	-1.4441	4.2865	0.0000	C	3.5740	-1.8337	0.0000	H	6.7744	-0.5883	0.0000
C	-2.8463	4.2861	0.0000	C	2.8993	-3.0780	0.0000	H	5.5264	1.5620	0.0000
C	-3.5366	3.0988	0.0000	C	3.6033	-4.2567	0.0000	H	1.7986	-3.0762	0.0000
C	-2.8479	1.8635	0.0000	C	5.0115	-4.2427	0.0000	H	3.0760	-5.2162	0.0000
C	-2.8578	-0.5878	0.0000	C	5.6899	-3.0489	0.0000	H	5.5577	-5.1916	0.0000
C	-3.5663	0.6148	0.0000	H	0.8989	-1.5287	0.0000	H	6.7857	-3.0293	0.0000
C	-4.9961	0.5882	0.0000	H	4.6310	3.0976	0.0000				

Table 3.654: Table of thermodynamic data as a function of temperature for Dinaphtho[1,2-*b*,2',1'-*n*]perylene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.973	595.024	595.024	∞
100	148.455	403.957	983.795	-57.984	627.396	691.154	-361.015
200	290.037	547.971	729.968	-36.399	610.304	761.725	-198.938
250	372.205	621.450	700.884	-19.858	602.229	800.513	-167.255
298.15	452.481	693.886	693.886	0.000	595.024	839.374	-147.052
300	455.532	696.694	693.895	0.840	594.758	840.888	-146.409
350	535.851	773.006	699.738	25.644	588.116	882.450	-131.696
400	610.497	849.504	713.680	54.330	582.359	924.889	-120.776
450	678.235	925.391	732.996	86.578	577.390	968.010	-112.361
500	738.855	1000.049	755.981	122.034	573.098	1011.674	-105.687
600	840.588	1144.119	808.772	201.208	566.174	1100.077	-95.768
700	921.033	1279.974	866.484	289.443	561.200	1189.488	-88.759
800	985.491	1407.321	926.217	384.883	557.955	1279.471	-83.539
900	1037.958	1526.527	986.368	486.143	556.214	1369.760	-79.497
1000	1081.249	1638.198	1046.028	592.170	555.774	1460.188	-76.271
1100	1117.363	1742.996	1104.675	702.154	556.384	1550.620	-73.631
1200	1147.755	1841.560	1162.016	815.452	557.866	1640.934	-71.427
1300	1173.522	1934.474	1217.897	931.551	559.991	1731.111	-69.555
1400	1195.509	2022.268	1272.245	1050.031	562.591	1821.110	-67.945
1500	1214.380	2105.409	1325.043	1170.549	565.565	1910.913	-66.543
1600	1230.666	2184.316	1376.303	1292.821	568.747	2000.498	-65.308
1700	1244.794	2259.358	1426.058	1416.610	572.044	2089.848	-64.212
1800	1257.109	2330.865	1474.354	1541.719	575.361	2179.087	-63.234
1900	1267.894	2399.129	1521.244	1667.981	578.659	2268.073	-62.352
2000	1277.382	2464.410	1566.782	1795.255	581.869	2356.921	-61.555
2100	1285.763	2526.940	1611.026	1923.421	584.891	2445.595	-60.830
2200	1293.198	2586.929	1654.031	2052.376	587.724	2534.132	-60.167
2300	1299.817	2644.563	1695.853	2182.033	590.363	2622.544	-59.559
2400	1305.733	2700.010	1736.545	2312.316	592.716	2710.783	-58.997
2500	1311.038	2753.422	1776.158	2443.159	594.799	2799.079	-58.482
2600	1315.811	2804.936	1814.742	2574.506	596.566	2887.144	-58.002
2700	1320.119	2854.678	1852.342	2706.306	598.022	2975.243	-57.558
2800	1324.020	2902.759	1889.003	2838.516	599.134	3063.322	-57.146
2900	1327.561	2949.283	1924.767	2971.098	599.864	3151.297	-56.760
3000	1330.785	2994.345	1959.672	3104.018	600.270	3239.289	-56.400
3100	1333.727	3038.030	1993.757	3237.246	600.249	3327.171	-56.061
3200	1336.419	3080.417	2027.056	3370.755	599.859	3415.158	-55.746
3300	1338.888	3121.579	2059.603	3504.522	599.074	3503.215	-55.450
3400	1341.157	3161.583	2091.428	3638.526	597.858	3591.187	-55.171
3500	1343.248	3200.491	2122.563	3772.747	596.217	3679.176	-54.908
3600	1345.177	3238.358	2153.033	3907.170	594.182	3767.336	-54.661
3700	1346.962	3275.240	2182.867	4041.778	591.710	3855.578	-54.430
3800	1348.615	3311.183	2212.089	4176.558	588.768	3943.815	-54.210
3900	1350.150	3346.234	2240.722	4311.497	585.409	4032.066	-54.002
4000	1351.576	3380.435	2268.789	4446.584	581.612	4120.592	-53.808
4100	1352.905	3413.825	2296.311	4581.809	577.331	4209.122	-53.624
4200	1354.144	3446.442	2323.308	4717.162	572.602	4297.750	-53.449
4300	1355.302	3478.320	2349.800	4852.635	567.407	4386.377	-53.283
4400	1356.385	3509.490	2375.803	4988.220	561.758	4475.251	-53.127
4500	1357.400	3539.983	2401.336	5123.910	555.674	4564.332	-52.980
4600	1358.352	3569.828	2426.415	5259.698	549.086	4653.565	-52.842
4700	1359.246	3599.051	2451.055	5395.579	542.014	4742.797	-52.709
4800	1360.086	3627.676	2475.271	5531.546	534.519	4832.323	-52.585
4900	1360.878	3655.728	2499.077	5667.594	526.504	4921.831	-52.466
5000	1361.624	3683.229	2522.486	5803.720	518.091	5011.754	-52.356

3.655. Dinaphtho[3,2,1-fg:1',2',3'-ij]pentaphene



Formula: $C_{36}H_{20}$
Mass: 452.544 g/mol
CAS Number: 128720-99-0
Point Group: C_2

Length: 15.81 Å
Width: 12.60 Å
Breadth: 7.358 Å
L/B Ratio: 1.255

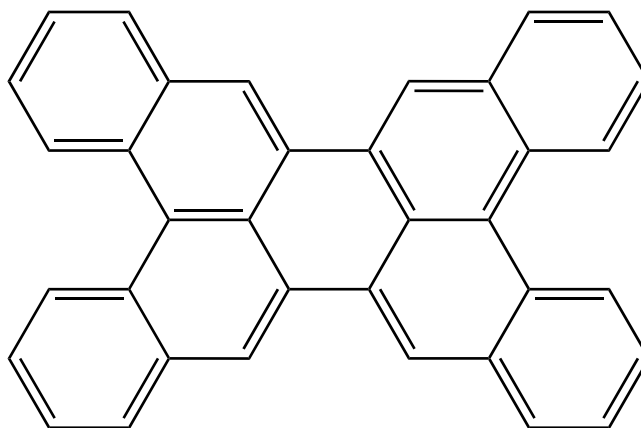
Cartesian coordinates:

C	-3.5104	3.8855	0.7917	C	1.4094	-2.0651	0.6754	H	4.6296	-0.9103	0.2620
C	-2.8290	2.6918	0.4855	C	2.8258	-2.0507	0.7072	H	0.8627	3.6373	-0.3684
C	-3.5544	1.5015	0.3092	C	3.5283	-0.9023	0.3005	H	2.9498	4.8032	-0.9304
C	-4.9558	1.5280	0.4328	C	2.8468	0.2650	0.0006	H	5.4254	4.8035	-1.1586
C	-5.6108	2.7041	0.7348	C	3.5582	1.4938	-0.3081	H	6.7078	2.7016	-0.8331
C	-4.8844	3.8884	0.9170	C	2.8356	2.6856	-0.4852	H	5.5153	0.5787	-0.2803
C	-2.8460	0.2711	0.0005	C	1.4074	2.6801	-0.3308	H	4.6306	-3.1801	1.1559
C	-1.4227	0.2647	0.0016	C	3.5198	3.8776	-0.7916	H	3.3985	-5.1419	2.0657
C	-0.7208	1.5258	0.1058	C	4.8938	3.8773	-0.9171	H	0.9212	-5.0969	2.2019
C	-1.4009	2.6831	0.3300	C	5.6174	2.6914	-0.7343	H	-0.3542	-3.1745	1.3093
C	-0.7169	-0.9342	-0.1586	C	4.9597	1.5170	-0.4315	H	0.3465	-3.1789	-1.3052
C	0.7150	-0.9359	0.1561	C	1.4439	-4.2480	1.7489	H	-0.9341	-5.0978	-2.1977
C	1.4235	0.2615	-0.0031	C	2.8605	-4.2655	1.6902	H	-3.4119	-5.1324	-2.0693
C	0.7245	1.5241	-0.1075	C	3.5352	-3.1927	1.1870	H	-4.6386	-3.1677	-1.1588
C	-3.5303	-0.8950	-0.2978	C	-1.4546	-4.2461	-1.7474	H	-5.5136	0.5908	0.2824
C	-2.8308	-2.0443	-0.7073	C	-2.8714	-4.2585	-1.6917	H	-6.7011	2.7168	0.8334
C	-1.4144	-2.0621	-0.6764	C	-3.5432	-3.1838	-1.1885	H	-5.4139	4.8160	1.1580
C	-0.7500	-3.1875	-1.2521	H	-4.6315	-0.9014	-0.2559	H	-2.9383	4.8098	0.9301
C	0.7421	-3.1874	1.2535	H	-0.8542	3.6391	0.3675				

Table 3.655: Table of thermodynamic data as a function of temperature for Dinaphtho[3,2,1-*fg*:1',2',3'-*ij*]pentaphene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.893	660.045	660.045	∞
100	147.523	391.137	972.914	-58.178	692.223	757.264	-395.540
200	291.161	535.281	718.095	-36.563	675.162	829.120	-216.540
250	373.899	609.073	688.878	-19.951	667.158	868.535	-181.467
298.15	454.623	681.847	681.847	0.000	660.045	907.984	-159.072
300	457.688	684.669	681.856	0.844	659.783	909.520	-158.358
350	538.325	761.339	687.727	25.764	653.257	951.675	-142.027
400	613.146	838.180	701.734	54.579	647.630	994.689	-129.890
450	680.943	914.384	721.137	86.961	642.794	1038.367	-120.528
500	741.544	989.327	744.222	122.553	638.638	1082.575	-113.094
600	843.111	1133.874	797.227	201.988	631.975	1172.026	-102.032
700	923.333	1270.101	855.152	290.464	627.243	1262.442	-94.203
800	987.570	1397.741	915.087	386.124	624.216	1353.396	-88.366
900	1039.834	1517.179	975.424	487.580	622.673	1444.631	-83.842
1000	1082.945	1629.039	1035.252	593.786	622.411	1535.984	-80.230
1100	1118.898	1733.991	1094.053	703.931	623.182	1627.325	-77.274
1200	1149.149	1832.682	1151.535	817.376	624.811	1718.532	-74.804
1300	1174.789	1925.703	1207.543	933.607	627.068	1809.592	-72.709
1400	1196.663	2013.586	1262.008	1052.209	629.789	1900.464	-70.906
1500	1215.435	2096.803	1314.912	1172.837	632.874	1991.131	-69.336
1600	1231.632	2175.775	1366.269	1295.210	636.157	2081.572	-67.955
1700	1245.680	2250.874	1416.114	1419.092	639.547	2171.774	-66.729
1800	1257.924	2322.429	1464.493	1544.286	642.949	2261.859	-65.636
1900	1268.645	2390.735	1511.459	1670.626	646.325	2351.686	-64.651
2000	1278.076	2456.053	1557.067	1797.972	649.607	2441.372	-63.761
2100	1286.406	2518.616	1601.376	1926.204	652.695	2530.880	-62.951
2200	1293.794	2578.634	1644.442	2055.222	655.591	2620.248	-62.211
2300	1300.371	2636.293	1686.321	2184.936	658.287	2709.488	-61.533
2400	1306.249	2691.763	1727.066	2315.273	660.693	2798.553	-60.908
2500	1311.520	2745.196	1766.729	2446.166	662.827	2887.673	-60.333
2600	1316.262	2796.728	1805.359	2577.559	664.640	2976.559	-59.799
2700	1320.542	2846.486	1843.004	2709.403	666.140	3065.478	-59.304
2800	1324.416	2894.582	1879.706	2841.654	667.293	3154.375	-58.844
2900	1327.934	2941.120	1915.508	2974.274	668.061	3243.168	-58.415
3000	1331.136	2986.194	1950.451	3107.230	668.503	3331.975	-58.014
3100	1334.058	3029.890	1984.570	3240.492	668.517	3420.672	-57.637
3200	1336.732	3072.287	2017.902	3374.033	668.158	3509.472	-57.285
3300	1339.184	3113.459	2050.480	3507.831	667.404	3598.342	-56.956
3400	1341.438	3153.471	2082.335	3641.863	666.216	3687.125	-56.645
3500	1343.514	3192.387	2113.498	3776.112	664.603	3775.926	-56.351
3600	1345.430	3230.262	2143.995	3910.561	662.594	3864.895	-56.077
3700	1347.202	3267.150	2173.854	4045.194	660.146	3953.946	-55.819
3800	1348.843	3303.099	2203.100	4179.997	657.228	4042.992	-55.574
3900	1350.367	3338.156	2231.757	4314.958	653.891	4132.051	-55.341
4000	1351.784	3372.363	2259.846	4450.067	650.116	4221.385	-55.124
4100	1353.103	3405.758	2287.389	4585.312	645.855	4310.721	-54.918
4200	1354.334	3438.380	2314.407	4720.684	641.145	4400.156	-54.723
4300	1355.483	3470.261	2340.918	4856.176	635.969	4489.589	-54.537
4400	1356.559	3501.436	2366.941	4991.779	630.337	4579.269	-54.362
4500	1357.566	3531.933	2392.492	5127.485	624.270	4669.155	-54.197
4600	1358.511	3561.781	2417.588	5263.290	617.699	4759.193	-54.041
4700	1359.399	3591.007	2442.244	5399.186	610.643	4849.229	-53.892
4800	1360.233	3619.636	2466.476	5535.168	603.163	4939.560	-53.752
4900	1361.019	3647.691	2490.297	5671.231	595.162	5029.872	-53.618
5000	1361.760	3675.195	2513.721	5807.370	586.763	5120.598	-53.493

3.656. Dinaphtho[1,2,3-*fg*:1',2',3'-*qr*]pentacene



Formula: $C_{36}H_{20}$
Mass: 452.544 g/mol
CAS Number: 36474-85-8
Point Group: D_2

Length: 15.53 Å
Width: 11.59 Å
Breadth: 6.148 Å
L/B Ratio: 1.340

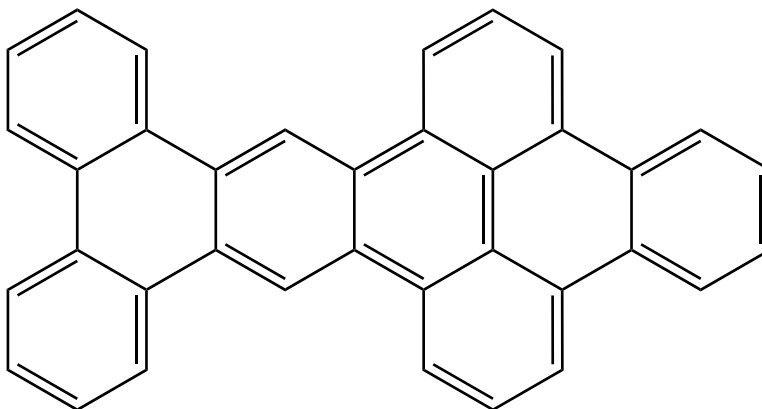
Cartesian coordinates:

C	0.7290	1.2339	0.0716	C	-2.8124	2.4190	-0.4541	H	-0.8611	3.3686	-0.2399
C	1.4059	2.4106	0.2393	C	-3.4559	3.6368	-0.7857	H	-0.8611	-3.3687	0.2399
C	1.4592	0.0000	0.0000	C	-4.7881	3.6524	-1.1109	H	-5.4892	-0.3350	0.8230
C	0.7290	-1.2339	-0.0715	C	-5.5106	2.4455	-1.1324	H	-6.5623	-2.4553	1.4373
C	1.4058	-2.4106	-0.2393	C	-4.9049	1.2643	-0.7812	H	-5.2909	-4.5897	1.3700
C	2.8624	0.0000	-0.0000	C	2.8123	2.4190	0.4548	H	-2.8694	-4.5628	0.7918
C	-0.7292	1.2339	-0.0707	C	3.5447	1.2162	0.3855	H	-2.8695	4.5628	-0.7918
C	-1.4061	2.4107	-0.2381	C	4.9049	1.2642	0.7808	H	-5.2909	4.5897	-1.3700
C	-0.7292	-1.2339	0.0707	C	5.5110	2.4455	1.1312	H	-6.5624	2.4553	-1.4373
C	-1.4593	0.0000	0.0000	C	4.7885	3.6524	1.1101	H	-5.4892	0.3350	-0.8230
C	-2.8626	-0.0000	0.0000	C	3.4560	3.6368	0.7861	H	5.4895	0.3351	0.8230
C	-1.4060	-2.4107	0.2381	C	3.5447	-1.2162	-0.3855	H	6.5628	2.4554	1.4357
C	-2.8124	-2.4190	0.4541	C	2.8123	-2.4190	-0.4548	H	5.2914	4.5897	1.3685
C	-3.5448	-1.2162	0.3854	C	3.4560	-3.6368	-0.7861	H	2.8694	4.5627	0.7927
C	-4.9049	-1.2643	0.7812	C	4.7885	-3.6524	-1.1101	H	2.8694	-4.5627	-0.7927
C	-5.5106	-2.4455	1.1324	C	5.5110	-2.4455	-1.1312	H	5.2914	-4.5897	-1.3685
C	-4.7881	-3.6524	1.1109	C	4.9049	-1.2642	-0.7808	H	6.5628	-2.4554	-1.4357
C	-3.4559	-3.6368	0.7857	H	0.8608	3.3685	0.2420	H	5.4895	-0.3351	-0.8230
C	-3.5448	1.2162	-0.3854	H	0.8608	-3.3685	-0.2420				

Table 3.656: Table of thermodynamic data as a function of temperature for Dinaphtho[1,2,3-*fg*:1',2',3'-*qr*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.374	646.385	646.385	∞
100	146.002	381.915	960.337	-57.842	678.899	744.861	-389.068
200	289.433	524.997	706.907	-36.382	661.683	817.698	-213.556
250	372.033	598.387	677.830	-19.861	653.588	857.637	-179.190
298.15	452.744	670.830	670.830	0.000	646.385	897.609	-157.254
300	455.811	673.640	670.839	0.840	646.119	899.166	-156.555
350	536.527	750.025	676.687	25.669	639.501	941.879	-140.565
400	611.475	826.635	690.644	54.396	633.787	985.464	-128.686
450	679.415	902.650	709.986	86.699	628.871	1029.725	-119.525
500	740.154	977.439	733.004	122.217	624.642	1074.524	-112.252
600	841.962	1121.755	785.877	201.526	617.853	1165.175	-101.435
700	922.365	1257.819	843.681	289.897	613.016	1256.812	-93.783
800	986.737	1385.339	903.506	385.467	609.899	1349.001	-88.079
900	1039.103	1504.686	963.746	486.845	608.278	1441.480	-83.660
1000	1082.295	1616.472	1023.490	592.982	607.947	1534.087	-80.131
1100	1118.315	1721.366	1082.215	703.066	608.657	1626.687	-77.243
1200	1148.621	1820.008	1139.629	816.455	610.230	1719.159	-74.832
1300	1174.310	1912.989	1195.576	932.636	612.437	1811.488	-72.785
1400	1196.227	2000.838	1249.987	1051.192	615.112	1903.633	-71.024
1500	1215.036	2084.027	1302.841	1171.778	618.155	1995.577	-69.491
1600	1231.266	2162.974	1354.153	1294.113	621.400	2087.297	-68.142
1700	1245.343	2238.051	1403.957	1417.960	624.755	2178.780	-66.944
1800	1257.614	2309.588	1452.299	1543.121	628.124	2270.148	-65.877
1900	1268.359	2377.878	1499.230	1669.432	631.471	2361.260	-64.914
2000	1277.811	2443.182	1544.807	1796.750	634.725	2452.233	-64.044
2100	1286.160	2505.733	1589.086	1924.957	637.788	2543.028	-63.253
2200	1293.566	2565.739	1632.125	2053.951	640.660	2633.685	-62.530
2300	1300.159	2623.389	1673.979	2183.643	643.334	2724.216	-61.868
2400	1306.051	2678.850	1714.700	2313.959	645.720	2814.571	-61.256
2500	1311.335	2732.275	1754.341	2444.833	647.834	2904.983	-60.695
2600	1316.088	2783.800	1792.951	2576.209	649.629	2995.161	-60.172
2700	1320.379	2833.552	1830.576	2708.036	651.112	3085.374	-59.689
2800	1324.263	2881.642	1867.260	2840.271	652.250	3175.564	-59.240
2900	1327.790	2928.175	1903.045	2972.876	653.003	3265.651	-58.820
3000	1331.000	2973.244	1937.971	3105.818	653.431	3355.753	-58.428
3100	1333.930	3016.936	1972.075	3239.067	653.432	3445.746	-58.059
3200	1336.611	3059.329	2005.393	3372.596	653.061	3535.841	-57.715
3300	1339.069	3100.497	2037.957	3506.382	652.295	3626.007	-57.394
3400	1341.329	3140.506	2069.799	3640.403	651.096	3716.086	-57.090
3500	1343.411	3179.418	2100.949	3774.642	649.472	3806.184	-56.803
3600	1345.332	3217.291	2131.435	3909.080	647.453	3896.450	-56.535
3700	1347.109	3254.176	2161.283	4043.703	644.996	3986.799	-56.282
3800	1348.755	3290.123	2190.519	4178.497	642.068	4077.142	-56.043
3900	1350.283	3325.178	2219.165	4313.450	638.723	4167.498	-55.816
4000	1351.703	3359.382	2247.245	4448.550	634.939	4258.131	-55.604
4100	1353.026	3392.776	2274.779	4583.788	630.670	4348.765	-55.403
4200	1354.260	3425.395	2301.787	4719.153	625.954	4439.498	-55.212
4300	1355.413	3457.275	2328.290	4854.637	620.770	4530.229	-55.030
4400	1356.492	3488.448	2354.304	4990.233	615.132	4621.208	-54.860
4500	1357.502	3518.944	2379.848	5125.933	609.058	4712.393	-54.699
4600	1358.449	3548.791	2404.936	5261.731	602.480	4803.730	-54.547
4700	1359.339	3578.015	2429.585	5397.621	595.418	4895.065	-54.401
4800	1360.176	3606.643	2453.810	5533.597	587.932	4986.695	-54.265
4900	1360.964	3634.697	2477.625	5669.655	579.925	5078.306	-54.134
5000	1361.707	3662.200	2501.042	5805.789	571.521	5170.332	-54.013

3.657. Tetrabenzo[*a,c,hi,qr*]pentacene



Formula: C₃₆H₂₀
Mass: 452.544 g/mol
CAS Number: 192-58-5
Point Group: C_{2v}

Length: 17.82 Å
Width: 11.65 Å
Breadth: 3.885 Å
L/B Ratio: 1.529

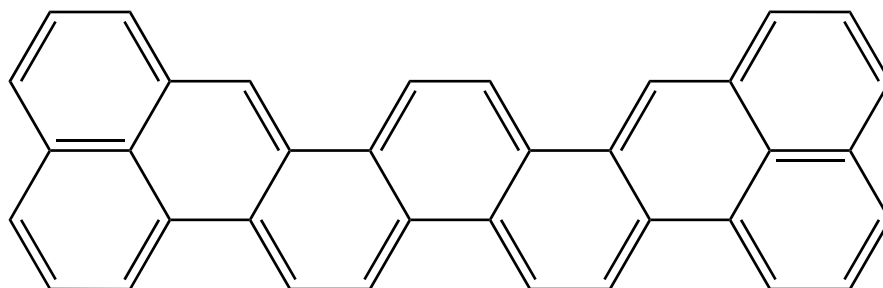
Cartesian coordinates:

C	-3.6759	2.8293	0.0000	C	0.0090	-0.7052	0.0000	H	-2.4756	4.6176	0.0000
C	-1.2721	2.8303	0.0000	C	1.2285	-1.3830	0.0000	H	-4.6292	-3.3787	0.0000
C	-2.4752	3.5227	0.0000	C	1.2276	1.3838	0.0000	H	-2.4725	-4.6191	0.0000
C	-3.6927	1.4300	0.0000	C	2.4486	0.7058	0.0000	H	-0.3154	-3.3788	0.0000
C	-3.6918	-1.4323	0.0000	C	2.4490	-0.7043	0.0000	H	-6.1734	2.4866	0.0000
C	-3.6740	-2.8316	0.0000	C	3.7096	1.4326	0.0000	H	-8.3268	1.2419	0.0000
C	-2.4729	-3.5242	0.0000	C	4.9259	0.7294	0.0000	H	-8.3261	-1.2469	0.0000
C	-1.2702	-2.8310	0.0000	C	6.1334	1.4499	0.0000	H	-6.1720	-2.4903	0.0000
C	-2.4728	0.7214	0.0000	C	6.1354	2.8310	0.0000	H	1.2296	-2.4900	0.0000
C	-2.4724	-0.7230	0.0000	C	4.9253	3.5304	0.0000	H	1.2281	2.4908	0.0000
C	-1.2526	-1.4336	0.0000	C	3.7300	2.8386	0.0000	H	7.0826	0.8924	0.0000
C	-1.2535	1.4329	0.0000	C	4.9264	-0.7264	0.0000	H	7.0826	3.3801	0.0000
C	-4.9521	-0.7038	0.0000	C	3.7105	-1.4304	0.0000	H	4.9279	4.6252	0.0000
C	-4.9525	0.7007	0.0000	C	3.7317	-2.8363	0.0000	H	2.7724	3.3818	0.0000
C	-6.1807	1.3858	0.0000	C	4.9274	-3.5274	0.0000	H	2.7745	-3.3801	0.0000
C	-7.3775	0.6966	0.0000	C	6.1371	-2.8273	0.0000	H	4.9306	-4.6222	0.0000
C	-7.3770	-0.7011	0.0000	C	6.1343	-1.4462	0.0000	H	7.0846	-3.3758	0.0000
C	-6.1799	-1.3896	0.0000	H	-4.6314	3.3757	0.0000	H	7.0831	-0.8881	0.0000
C	0.0086	0.7053	0.0000	H	-0.3176	3.3787	0.0000				

Table 3.657: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,c,hi,qr*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.994	575.892	575.892	∞
100	148.932	405.220	984.287	-57.907	608.341	671.973	-350.995
200	289.614	549.247	730.872	-36.325	591.247	742.411	-193.894
250	371.419	622.591	701.850	-19.815	583.141	781.139	-163.207
298.15	451.478	694.868	694.868	0.000	575.892	819.949	-143.649
300	454.523	697.670	694.876	0.838	575.624	821.461	-143.026
350	534.756	773.818	700.707	25.589	568.928	862.979	-128.790
400	609.408	850.170	714.620	54.220	563.117	905.381	-118.228
450	677.195	925.931	733.899	86.415	558.094	948.471	-110.093
500	737.882	1000.483	756.842	121.821	553.752	992.112	-103.643
600	839.745	1144.387	809.547	200.904	546.738	1080.480	-94.062
700	920.288	1280.120	867.178	289.059	541.685	1169.871	-87.295
800	984.817	1407.373	926.836	384.429	538.369	1259.844	-82.258
900	1037.336	1526.502	986.920	485.624	536.563	1350.131	-78.358
1000	1080.671	1638.110	1046.518	591.591	536.063	1440.565	-75.246
1100	1116.823	1742.855	1105.110	701.519	536.617	1531.009	-72.700
1200	1147.251	1841.373	1162.402	814.766	538.047	1621.339	-70.574
1300	1173.052	1934.249	1218.237	930.815	540.123	1711.537	-68.769
1400	1195.070	2022.008	1272.544	1049.250	542.678	1801.560	-67.216
1500	1213.971	2105.120	1325.303	1169.726	545.609	1891.391	-65.863
1600	1230.286	2184.001	1376.528	1291.958	548.752	1981.005	-64.672
1700	1244.439	2259.022	1426.251	1415.711	552.012	2070.388	-63.614
1800	1256.779	2330.509	1474.517	1540.786	555.295	2159.662	-62.670
1900	1267.586	2398.756	1521.379	1667.016	558.561	2248.684	-61.819
2000	1277.094	2464.021	1566.891	1794.260	561.741	2337.571	-61.050
2100	1285.495	2526.538	1611.111	1922.398	564.735	2426.284	-60.349
2200	1292.947	2586.515	1654.093	2051.327	567.543	2514.862	-59.709
2300	1299.582	2644.138	1695.894	2180.960	570.157	2603.316	-59.122
2400	1305.512	2699.575	1736.567	2311.220	572.487	2691.598	-58.580
2500	1310.831	2752.978	1776.162	2442.042	574.549	2779.938	-58.082
2600	1315.617	2804.485	1814.728	2573.368	576.296	2868.048	-57.619
2700	1319.937	2854.219	1852.312	2705.150	577.733	2956.192	-57.190
2800	1323.847	2902.294	1888.958	2837.342	578.828	3044.317	-56.791
2900	1327.398	2948.813	1924.707	2969.907	579.541	3132.340	-56.418
3000	1330.631	2993.869	1959.598	3102.811	579.931	3220.378	-56.071
3100	1333.582	3037.549	1993.670	3236.024	579.896	3308.309	-55.743
3200	1336.282	3079.931	2026.957	3369.519	579.491	3396.344	-55.438
3300	1338.758	3121.090	2059.492	3503.273	578.692	3484.450	-55.153
3400	1341.034	3161.090	2091.306	3637.264	577.464	3572.470	-54.883
3500	1343.130	3199.994	2122.430	3771.474	575.811	3660.510	-54.629
3600	1345.065	3237.858	2152.890	3905.885	573.764	3748.719	-54.391
3700	1346.855	3274.736	2182.714	4040.482	571.281	3837.011	-54.168
3800	1348.514	3310.677	2211.927	4175.251	568.329	3925.298	-53.956
3900	1350.053	3345.725	2240.551	4310.181	564.960	4013.600	-53.755
4000	1351.484	3379.924	2268.609	4445.258	561.154	4102.178	-53.568
4100	1352.817	3413.312	2296.123	4580.474	556.864	4190.758	-53.390
4200	1354.060	3445.927	2323.113	4715.819	552.126	4279.437	-53.221
4300	1355.221	3477.802	2349.597	4851.283	546.923	4368.116	-53.061
4400	1356.308	3508.971	2375.594	4986.860	541.266	4457.042	-52.911
4500	1357.325	3539.462	2401.120	5122.543	535.174	4546.175	-52.770
4600	1358.280	3569.306	2426.192	5258.323	528.579	4635.461	-52.636
4700	1359.177	3598.527	2450.825	5394.197	521.500	4724.744	-52.509
4800	1360.020	3627.151	2475.035	5530.157	513.999	4814.323	-52.389
4900	1360.814	3655.202	2498.835	5666.199	505.977	4903.884	-52.275
5000	1361.563	3682.702	2522.238	5802.318	497.558	4993.860	-52.169

3.658. Dinaphtho[1,8-*bc*:1',8'-*mn*]picene



Formula: $C_{36}H_{20}$
Mass: 452.544 g/mol
CAS Number: 128721-02-8
Point Group: C_{2v}

Length: 20.29 Å
Width: 9.188 Å
Breadth: 3.884 Å
L/B Ratio: 2.209

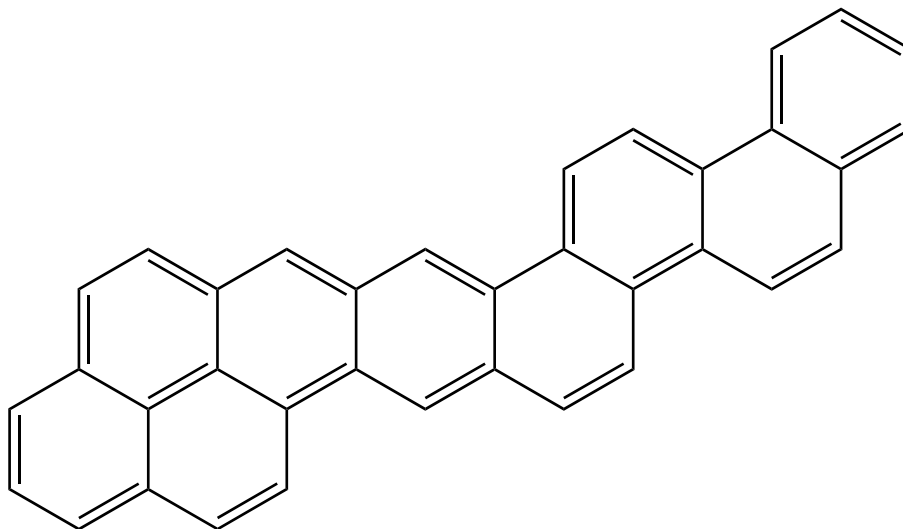
Cartesian coordinates:

C	-5.0287	-1.4957	0.0000	C	5.7372	-0.2607	0.0000	H	5.2139	3.1198	0.0000
C	-3.5859	-1.4701	0.0000	C	5.0283	-1.4969	0.0000	H	5.1875	-3.6445	0.0000
C	-2.8856	-0.3040	0.0000	C	3.5856	-1.4710	0.0000	H	7.6650	-3.6483	0.0000
C	-3.5756	0.9777	0.0000	C	5.7545	2.1606	0.0000	H	8.9304	-1.5107	0.0000
C	-5.0358	0.9824	0.0000	C	7.1638	2.1491	0.0000	H	3.0482	-2.4337	0.0000
C	-5.7373	-0.2594	0.0000	C	7.8515	0.9644	0.0000	H	3.3951	3.1039	0.0000
C	-2.8636	2.1398	0.0000	C	7.1478	-0.2695	0.0000	H	0.9069	3.1018	0.0000
C	-1.4386	2.1383	0.0000	C	5.7261	-2.6902	0.0000	H	-1.2420	-2.4333	0.0000
C	-0.7291	0.9710	0.0000	C	7.1339	-2.6905	0.0000	H	1.2414	-2.4336	0.0000
C	-1.4248	-0.3025	0.0000	C	7.8346	-1.5109	0.0000	H	-0.9061	3.1021	0.0000
C	0.7293	0.9708	0.0000	C	-7.1479	-0.2678	0.0000	H	-3.3943	3.1048	0.0000
C	1.4247	-0.3029	0.0000	C	-7.8514	0.9662	0.0000	H	-3.0487	-2.4329	0.0000
C	0.7118	-1.4681	0.0000	C	-7.1634	2.1508	0.0000	H	-5.2134	3.1211	0.0000
C	-0.7122	-1.4680	0.0000	C	-5.7541	2.1620	0.0000	H	-7.7008	3.1049	0.0000
C	1.4392	2.1379	0.0000	C	-5.7267	-2.6888	0.0000	H	-8.9470	0.9522	0.0000
C	2.8641	2.1391	0.0000	C	-7.1344	-2.6889	0.0000	H	-8.9307	-1.5087	0.0000
C	3.5759	0.9768	0.0000	C	-7.8349	-1.5091	0.0000	H	-7.6658	-3.6465	0.0000
C	2.8855	-0.3048	0.0000	H	8.9472	0.9502	0.0000	H	-5.1883	-3.6433	0.0000
C	5.0361	0.9812	0.0000	H	7.7014	3.1032	0.0000				

Table 3.658: Table of thermodynamic data as a function of temperature for Dinaphtho[1,8-*bc*:1',8'-*mn*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-67.241	736.558	736.558	∞
100	147.206	404.051	986.726	-58.268	768.646	832.395	-434.790
200	291.700	547.997	731.374	-36.675	751.563	902.978	-235.829
250	375.103	621.989	702.062	-20.018	743.603	941.752	-196.764
298.15	456.171	695.008	695.008	0.000	736.558	980.573	-171.789
300	459.246	697.839	695.016	0.847	736.299	982.085	-170.993
350	540.054	774.763	700.907	25.850	729.856	1023.575	-152.757
400	614.950	851.841	714.959	54.753	724.317	1065.911	-139.191
450	682.761	928.259	734.423	87.226	719.572	1108.902	-128.715
500	743.335	1003.392	757.576	122.908	715.506	1152.411	-120.389
600	844.774	1148.255	810.727	202.517	709.017	1240.438	-107.988
700	924.820	1284.726	868.797	291.150	704.442	1329.404	-99.199
800	988.874	1412.553	928.866	386.950	701.555	1418.886	-92.642
900	1040.967	1532.135	989.326	488.528	700.134	1508.632	-87.557
1000	1083.928	1644.105	1049.266	594.839	699.977	1598.484	-83.495
1100	1119.752	1749.145	1108.167	705.076	700.840	1688.313	-80.170
1200	1149.893	1847.905	1165.738	818.601	702.549	1778.001	-77.393
1300	1175.441	1940.982	1221.827	934.902	704.876	1867.536	-75.037
1400	1197.238	2028.911	1276.365	1053.564	707.658	1956.877	-73.010
1500	1215.943	2112.165	1329.334	1174.247	710.796	2046.010	-71.247
1600	1232.085	2191.168	1380.751	1296.668	714.127	2134.914	-69.696
1700	1246.085	2266.293	1430.651	1420.592	717.560	2223.575	-68.321
1800	1258.288	2337.871	1479.079	1545.825	721.001	2312.117	-67.094
1900	1268.975	2406.195	1526.090	1672.199	724.411	2400.399	-65.990
2000	1278.374	2471.529	1571.741	1799.577	727.725	2488.538	-64.993
2100	1286.678	2534.106	1616.088	1927.838	730.842	2576.497	-64.086
2200	1294.043	2594.136	1659.190	2056.881	733.763	2664.316	-63.258
2300	1300.600	2651.806	1701.102	2186.619	736.483	2752.006	-62.499
2400	1306.459	2707.285	1741.878	2316.978	738.912	2839.519	-61.799
2500	1311.714	2760.726	1781.569	2447.891	741.065	2927.085	-61.157
2600	1316.442	2812.266	1820.226	2579.303	742.897	3014.418	-60.559
2700	1320.709	2862.030	1857.895	2711.164	744.414	3101.783	-60.006
2800	1324.572	2910.132	1894.621	2843.431	745.583	3189.126	-59.493
2900	1328.079	2956.675	1930.445	2976.067	746.367	3276.363	-59.012
3000	1331.272	3001.754	1965.408	3109.037	746.823	3363.615	-58.565
3100	1334.185	3045.454	1999.547	3242.312	746.850	3450.755	-58.144
3200	1336.851	3087.856	2032.898	3375.866	746.503	3537.999	-57.751
3300	1339.296	3129.031	2065.493	3509.675	745.760	3625.311	-57.383
3400	1341.544	3169.047	2097.365	3643.718	744.584	3712.537	-57.035
3500	1343.614	3207.965	2128.543	3777.977	742.981	3799.780	-56.707
3600	1345.524	3245.843	2159.055	3912.436	740.981	3887.191	-56.401
3700	1347.291	3282.733	2188.928	4047.078	738.543	3974.685	-56.111
3800	1348.929	3318.685	2218.188	4181.890	735.633	4062.172	-55.837
3900	1350.448	3353.744	2246.857	4316.859	732.305	4149.672	-55.577
4000	1351.861	3387.953	2274.959	4451.976	728.537	4237.447	-55.334
4100	1353.176	3421.350	2302.514	4587.228	724.284	4325.225	-55.103
4200	1354.404	3453.973	2329.543	4722.608	719.582	4413.100	-54.884
4300	1355.550	3485.856	2356.064	4858.106	714.412	4500.973	-54.675
4400	1356.622	3517.032	2382.097	4993.716	708.787	4589.094	-54.478
4500	1357.627	3547.531	2407.658	5129.429	702.726	4677.420	-54.293
4600	1358.569	3577.380	2432.763	5265.239	696.161	4765.899	-54.117
4700	1359.455	3606.608	2457.429	5401.141	689.110	4854.374	-53.949
4800	1360.287	3635.238	2481.669	5537.128	681.636	4943.145	-53.791
4900	1361.071	3663.294	2505.499	5673.196	673.640	5031.897	-53.640
5000	1361.809	3690.799	2528.931	5809.341	665.247	5121.063	-53.498

3.659. Pyreno[2,1-*b*]picene



Formula: C₃₆H₂₀
Mass: 452.544 g/mol
CAS Number: 119000-35-0
Point Group: C_s

Length: 22.18 Å
Width: 9.539 Å
Breadth: 3.885 Å
L/B Ratio: 2.325

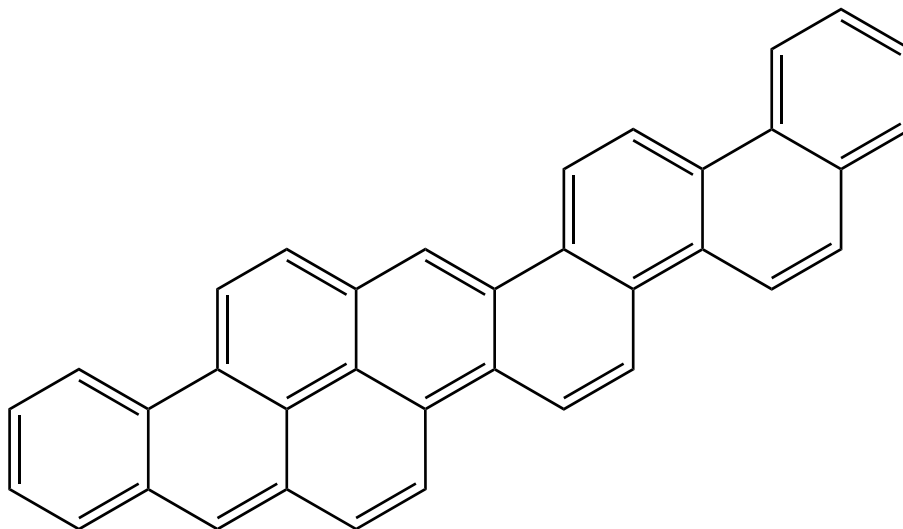
Cartesian coordinates:

C	8.0819	-1.0704	0.0000	C	-0.1263	1.4451	0.0000	H	8.1880	2.3400	0.0000
C	8.6072	0.2277	0.0000	C	-1.0402	2.5573	0.0000	H	5.9082	3.2819	0.0000
C	7.7724	1.3260	0.0000	C	-2.3766	2.3572	0.0000	H	3.4396	2.9384	0.0000
C	6.3740	1.1542	0.0000	C	-2.0821	-0.0738	0.0000	H	2.1039	-2.8733	0.0000
C	5.4810	2.2726	0.0000	C	-2.9378	1.0312	0.0000	H	4.3743	-3.7961	0.0000
C	4.1350	2.0847	0.0000	C	-3.9833	-1.5736	0.0000	H	6.8276	-3.4506	0.0000
C	3.5688	0.7710	0.0000	C	-2.6308	-1.3819	0.0000	H	1.6569	2.6765	0.0000
C	2.5242	-1.8599	0.0000	C	-4.8734	-0.4688	0.0000	H	-0.1623	-1.9773	0.0000
C	4.4183	-0.3358	0.0000	C	-4.3544	0.8332	0.0000	H	-0.6211	3.5701	0.0000
C	3.8808	-1.6684	0.0000	C	-5.2591	1.9466	0.0000	H	-3.0759	3.2071	0.0000
C	4.8025	-2.7870	0.0000	C	-6.6021	1.7632	0.0000	H	-4.4121	-2.5876	0.0000
C	6.1366	-2.5997	0.0000	C	-6.3033	-0.6719	0.0000	H	-1.9383	-2.2377	0.0000
C	6.7087	-1.2698	0.0000	C	-7.1598	0.4431	0.0000	H	-4.8276	2.9591	0.0000
C	5.8373	-0.1493	0.0000	C	-8.5599	0.2508	0.0000	H	-7.2875	2.6185	0.0000
C	1.6294	-0.7482	0.0000	C	-9.0855	-1.0195	0.0000	H	-9.2186	1.1267	0.0000
C	2.1434	0.5733	0.0000	C	-8.2321	-2.1375	0.0000	H	-10.1699	-1.1706	0.0000
C	1.2483	1.6530	0.0000	C	-6.8681	-1.9677	0.0000	H	-8.6635	-3.1438	0.0000
C	0.2404	-0.9514	0.0000	H	8.7608	-1.9307	0.0000	H	-6.1896	-2.8345	0.0000
C	-0.6441	0.1215	0.0000	H	9.6937	0.3658	0.0000				

Table 3.659: Table of thermodynamic data as a function of temperature for Pyreno[2,1-*b*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _p ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _r)	Δ _f <i>H</i> ^o	Δ _f <i>G</i> ^o	log <i>K</i> _f
0	0.0	0.0	∞	-66.420	576.943	576.943	∞
100	144.411	404.300	981.073	-57.677	609.622	673.346	-351.713
200	288.773	546.233	728.113	-36.376	592.247	744.015	-194.313
250	372.071	619.562	699.032	-19.868	584.140	782.895	-163.574
298.15	452.924	692.030	692.030	0.000	576.943	821.847	-143.981
300	455.989	694.841	692.039	0.841	576.678	823.364	-143.357
350	536.549	771.244	697.889	25.675	570.066	865.017	-129.094
400	611.253	847.841	711.848	54.397	564.346	907.541	-118.510
450	678.966	923.817	731.188	86.683	559.414	950.743	-110.357
500	739.534	998.549	754.200	122.174	555.158	994.484	-103.891
600	841.171	1142.733	807.048	201.411	548.296	1083.031	-94.284
700	921.564	1278.674	864.815	289.701	543.378	1172.576	-87.497
800	986.002	1406.090	924.598	385.194	540.185	1262.685	-82.443
900	1038.462	1525.356	984.796	486.504	538.495	1353.094	-78.530
1000	1081.749	1637.079	1044.498	592.581	538.104	1443.637	-75.406
1100	1117.855	1741.925	1103.185	702.615	538.764	1534.179	-72.851
1200	1148.236	1840.531	1160.563	815.962	540.295	1624.597	-70.715
1300	1173.987	1933.484	1216.478	932.108	542.467	1714.875	-68.903
1400	1195.955	2021.310	1270.858	1050.633	545.113	1804.972	-67.343
1500	1214.806	2104.482	1323.685	1171.195	548.130	1894.869	-65.984
1600	1231.071	2183.416	1374.973	1293.509	551.354	1984.545	-64.787
1700	1245.177	2258.482	1424.754	1417.337	554.690	2073.984	-63.724
1800	1257.471	2330.010	1473.075	1542.484	558.045	2163.309	-62.776
1900	1268.235	2398.293	1519.987	1668.781	561.378	2252.380	-61.921
2000	1277.703	2463.591	1565.547	1796.087	564.621	2341.311	-61.148
2100	1286.066	2526.137	1609.811	1924.284	567.673	2430.066	-60.443
2200	1293.482	2586.139	1652.835	2053.269	570.536	2518.682	-59.800
2300	1300.085	2643.785	1694.675	2182.954	573.203	2607.173	-59.210
2400	1305.985	2699.243	1735.384	2313.263	575.582	2695.490	-58.665
2500	1311.276	2752.665	1775.013	2444.130	577.690	2783.862	-58.164
2600	1316.036	2804.189	1813.612	2575.500	579.479	2872.001	-57.698
2700	1320.331	2853.938	1851.226	2707.322	580.957	2960.175	-57.267
2800	1324.220	2902.027	1887.901	2839.553	582.090	3048.327	-56.866
2900	1327.750	2948.558	1923.677	2972.154	582.839	3136.376	-56.491
3000	1330.964	2993.626	1958.595	3105.092	583.263	3224.439	-56.141
3100	1333.897	3037.317	1992.692	3238.338	583.261	3312.393	-55.812
3200	1336.581	3079.709	2026.002	3371.863	582.887	3400.451	-55.506
3300	1339.041	3120.876	2058.559	3505.646	582.117	3488.579	-55.218
3400	1341.303	3160.885	2090.395	3639.665	580.916	3576.620	-54.947
3500	1343.387	3199.796	2121.539	3773.901	579.290	3664.680	-54.691
3600	1345.310	3237.668	2152.019	3908.337	577.268	3752.908	-54.452
3700	1347.088	3274.552	2181.861	4042.958	574.809	3841.219	-54.227
3800	1348.735	3310.499	2211.091	4177.750	571.879	3929.525	-54.014
3900	1350.265	3345.553	2239.732	4312.701	568.532	4017.844	-53.812
4000	1351.686	3379.757	2267.807	4447.800	564.747	4106.439	-53.623
4100	1353.010	3413.150	2295.337	4583.035	560.476	4195.036	-53.444
4200	1354.245	3445.769	2322.341	4718.399	555.758	4283.731	-53.275
4300	1355.399	3477.649	2348.839	4853.882	550.573	4372.425	-53.113
4400	1356.478	3508.822	2374.850	4989.476	544.933	4461.366	-52.962
4500	1357.489	3539.317	2400.389	5125.175	538.858	4550.514	-52.820
4600	1358.437	3569.164	2425.474	5260.972	532.279	4639.814	-52.686
4700	1359.328	3598.388	2450.120	5396.861	525.216	4729.112	-52.557
4800	1360.165	3627.015	2474.341	5532.836	517.729	4818.704	-52.437
4900	1360.954	3655.069	2498.153	5668.892	509.721	4908.278	-52.322
5000	1361.697	3682.572	2521.567	5805.025	501.316	4998.267	-52.215

3.660. Dibenzo[*b,tuv*]naphtho[2,1-*m*]picene



Formula: C₃₆H₂₀
Mass: 452.544 g/mol
CAS Number: 13354-54-6
Point Group: C_s

Length: 22.29 Å
Width: 9.202 Å
Breadth: 3.886 Å
L/B Ratio: 2.423

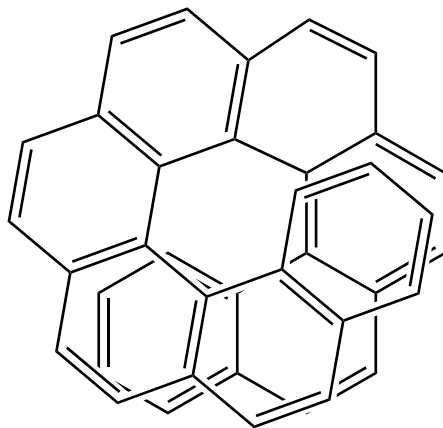
Cartesian coordinates:

C	8.1787	-1.7800	0.0000	C	0.0918	1.1290	0.0000	H	8.3998	1.6275	0.0000
C	8.7568	-0.4880	0.0000	C	-0.7632	2.2802	0.0000	H	6.3546	-2.9258	0.0000
C	7.9608	0.6232	0.0000	C	-2.1117	2.1546	0.0000	H	6.1840	2.6380	0.0000
C	6.8198	-1.9281	0.0000	C	-1.9358	-0.2816	0.0000	H	3.9574	3.6708	0.0000
C	5.9634	-0.7921	0.0000	C	-2.7379	0.8645	0.0000	H	1.4852	3.4411	0.0000
C	6.5424	0.4963	0.0000	C	-3.9129	-1.6839	0.0000	H	-0.1381	-2.2911	0.0000
C	5.7173	1.6451	0.0000	C	-2.5543	-1.5614	0.0000	H	2.0884	-3.3257	0.0000
C	4.3430	1.5222	0.0000	C	-4.7484	-0.5347	0.0000	H	4.5676	-3.0970	0.0000
C	3.4838	2.6822	0.0000	C	-4.1650	0.7380	0.0000	H	-0.2861	3.2722	0.0000
C	2.1397	2.5560	0.0000	C	-5.0105	1.8959	0.0000	H	-2.7623	3.0425	0.0000
C	1.5024	1.2616	0.0000	C	-6.3617	1.7808	0.0000	H	-4.3933	-2.6745	0.0000
C	0.3304	-1.2938	0.0000	C	-6.1858	-0.6658	0.0000	H	-1.9095	-2.4535	0.0000
C	2.3111	0.1122	0.0000	C	-6.9850	0.4912	0.0000	H	-4.5275	2.8849	0.0000
C	1.7135	-1.1763	0.0000	C	-8.3935	0.3694	0.0000	H	-7.0026	2.6700	0.0000
C	2.5635	-2.3380	0.0000	C	-8.9822	-0.8725	0.0000	H	-9.0070	1.2775	0.0000
C	3.9107	-2.2133	0.0000	C	-8.1860	-2.0325	0.0000	H	-10.0728	-0.9690	0.0000
C	4.5427	-0.9216	0.0000	C	-6.8156	-1.9319	0.0000	H	-8.6679	-3.0156	0.0000
C	3.7424	0.2266	0.0000	H	8.8343	-2.6569	0.0000	H	-6.1814	-2.8315	0.0000
C	-0.4936	-0.1565	0.0000	H	9.8475	-0.3929	0.0000				

Table 3.660: Table of thermodynamic data as a function of temperature for Dibenzob[*b,tuv*]naphtho[2,1-*m*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-66.586	582.311	582.311	∞
100	145.802	408.382	985.530	-57.715	614.952	678.268	-354.284
200	288.886	550.920	732.589	-36.334	597.657	748.487	-195.481
250	371.604	624.209	703.549	-19.835	589.540	787.134	-164.459
298.15	452.060	696.559	696.559	0.000	582.311	825.864	-144.685
300	455.114	699.364	696.567	0.839	582.044	827.373	-144.055
350	535.420	775.612	702.406	25.622	575.381	868.804	-129.659
400	609.987	852.048	716.336	54.285	569.601	911.114	-118.977
450	677.644	927.870	735.636	86.505	564.604	954.109	-110.748
500	738.205	1002.463	758.602	121.931	560.281	997.651	-104.222
600	839.901	1146.409	811.348	201.037	553.290	1085.819	-94.527
700	920.381	1282.160	869.011	289.204	548.249	1175.006	-87.678
800	984.908	1409.425	928.696	384.583	544.942	1264.775	-82.580
900	1037.451	1528.566	988.802	485.787	543.146	1354.856	-78.632
1000	1080.814	1640.187	1048.420	591.768	542.659	1445.083	-75.482
1100	1116.992	1744.947	1107.028	701.711	543.228	1535.319	-72.905
1200	1147.438	1843.481	1164.335	814.976	544.676	1625.438	-70.752
1300	1173.251	1936.372	1220.184	931.045	546.772	1715.425	-68.925
1400	1195.275	2024.147	1274.504	1049.500	549.346	1805.235	-67.353
1500	1214.178	2107.273	1327.276	1169.996	552.299	1894.851	-65.983
1600	1230.490	2186.168	1378.512	1292.249	555.462	1984.250	-64.778
1700	1244.639	2261.200	1428.246	1416.022	558.743	2073.415	-63.707
1800	1256.973	2332.699	1476.523	1541.116	562.045	2162.471	-62.752
1900	1267.773	2400.955	1523.395	1667.365	565.330	2251.274	-61.891
2000	1277.274	2466.230	1568.916	1794.628	568.529	2339.940	-61.112
2100	1285.667	2528.756	1613.145	1922.783	571.540	2428.431	-60.403
2200	1293.110	2588.740	1656.136	2051.730	574.364	2516.787	-59.755
2300	1299.738	2646.371	1697.945	2181.378	576.995	2605.019	-59.161
2400	1305.661	2701.814	1738.625	2311.654	579.341	2693.077	-58.612
2500	1310.972	2755.224	1778.228	2442.490	581.417	2781.193	-58.109
2600	1315.751	2806.736	1816.801	2573.830	583.177	2869.077	-57.639
2700	1320.064	2856.475	1854.392	2705.625	584.628	2956.997	-57.205
2800	1323.969	2904.554	1891.044	2837.830	585.734	3044.896	-56.802
2900	1327.514	2951.077	1926.799	2970.407	586.459	3132.692	-56.425
3000	1330.741	2996.137	1961.696	3103.322	586.861	3220.504	-56.073
3100	1333.686	3039.820	1995.773	3236.545	586.836	3308.207	-55.742
3200	1336.381	3082.206	2029.065	3370.051	586.442	3396.015	-55.433
3300	1338.853	3123.367	2061.605	3503.814	585.653	3483.893	-55.144
3400	1341.124	3163.370	2093.425	3637.815	584.433	3571.686	-54.871
3500	1343.217	3202.277	2124.553	3772.033	582.790	3659.497	-54.614
3600	1345.148	3240.144	2155.018	3906.453	580.751	3747.478	-54.373
3700	1346.934	3277.024	2184.846	4041.058	578.277	3835.542	-54.147
3800	1348.589	3312.967	2214.063	4175.835	575.332	3923.600	-53.933
3900	1350.125	3348.017	2242.691	4310.772	571.970	4011.673	-53.729
4000	1351.553	3382.217	2270.753	4445.856	568.171	4100.021	-53.540
4100	1352.883	3415.607	2298.271	4581.079	563.888	4188.372	-53.359
4200	1354.123	3448.224	2325.264	4716.430	559.157	4276.822	-53.189
4300	1355.282	3480.101	2351.752	4851.901	553.960	4365.271	-53.026
4400	1356.366	3511.270	2377.751	4987.484	548.309	4453.967	-52.874
4500	1357.382	3541.763	2403.281	5123.172	542.223	4542.870	-52.731
4600	1358.334	3571.608	2428.356	5258.958	535.633	4631.926	-52.596
4700	1359.229	3600.830	2452.992	5394.837	528.560	4720.979	-52.467
4800	1360.071	3629.455	2477.205	5530.802	521.063	4810.327	-52.346
4900	1360.863	3657.507	2501.007	5666.849	513.046	4899.658	-52.230
5000	1361.609	3685.008	2524.413	5802.973	504.632	4989.403	-52.123

3.661. Diphenanthro[3,4-c:4',3'-g]phenanthrene



Formula: $C_{38}H_{22}$
Mass: 478.581 g/mol
CAS Number: 20495-14-1
Point Group: C_2

Length: 12.83 Å
Width: 11.44 Å
Breadth: 8.253 Å
L/B Ratio: 1.121

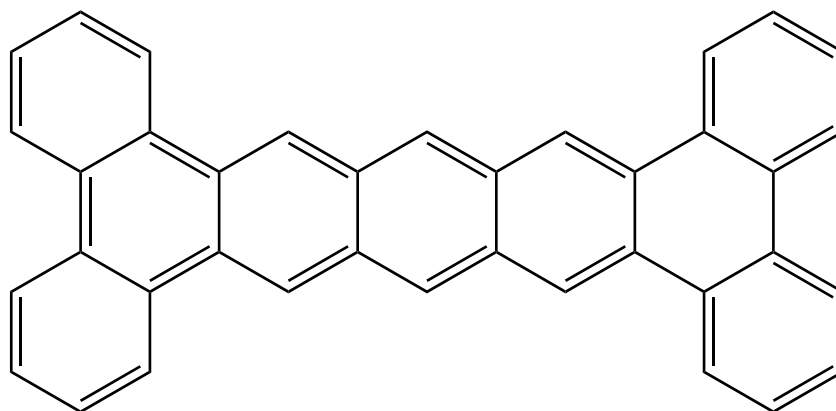
Cartesian coordinates:

C	2.4422	0.6637	-1.3699	C	0.9495	2.8832	1.0234	H	1.9485	-2.8243	2.9740
C	1.7285	-0.5575	-1.4100	C	0.3759	1.6657	0.6170	H	3.1954	-0.6982	3.3529
C	2.4733	-1.7548	-1.3914	C	2.0007	2.8959	1.9882	H	3.3367	1.7013	3.1623
C	3.8752	-1.7177	-1.2112	C	2.4595	1.7257	2.5060	H	2.4560	3.8546	2.2607
C	4.5335	-0.5154	-1.1256	C	1.7600	0.5083	2.2488	H	0.9297	5.0517	0.8320
C	3.8098	0.6848	-1.2328	C	0.5949	0.5123	1.4605	H	-0.9234	5.0519	-0.8379
C	0.2936	-0.6163	-1.5938	C	-0.2940	-0.6154	1.5938	H	-2.4550	3.8545	-2.2610
C	-0.2462	-1.8258	-2.0551	C	0.2454	-1.8251	2.0550	H	-3.3366	1.7012	-3.1618
C	0.5201	-3.0342	-1.9996	C	1.5479	-1.8641	2.6301	H	-3.1968	-0.6984	-3.3512
C	1.8228	-3.0084	-1.6260	C	2.2438	-0.7079	2.8097	H	-4.4312	-2.6585	1.1590
C	-1.5489	-1.8645	-2.6297	C	-0.5214	-3.0331	1.9995	H	-1.8924	1.6115	1.4594
C	-2.2449	-0.7083	-2.8085	C	-1.8243	-3.0067	1.6269	H	-4.3439	1.6427	1.2063
C	-1.7606	0.5078	-2.2478	C	-2.4743	-1.7528	1.3923	H	-5.6195	-0.4790	0.9907
C	-0.5950	0.5115	-1.4600	C	-1.7289	-0.5559	1.4104	H	-1.9496	-2.8247	-2.9738
C	-2.4594	1.7254	-2.5055	C	-2.4419	0.6657	1.3700	H	0.0247	-3.9772	-2.2577
C	-1.9995	2.8957	-1.9890	C	-3.8094	0.6874	1.2328	H	2.4091	-3.9303	-1.5425
C	-0.9473	2.8831	-1.0251	C	-4.5338	-0.5124	1.1260	H	4.4295	-2.6615	-1.1571
C	-0.3749	1.6655	-0.6176	C	-3.8762	-1.7150	1.2122	H	5.6192	-0.4825	-0.9902
C	-0.4926	4.1144	-0.4687	H	-0.0259	-3.9763	2.2568	H	4.3448	1.6397	-1.2066
C	0.4969	4.1143	0.4649	H	-2.4114	-3.9282	1.5451	H	1.8933	1.6098	-1.4593

Table 3.661: Table of thermodynamic data as a function of temperature for Diphenanthro[3,4-c:4',3'-g]phenanthrene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-71.500	755.233	755.233	∞
100	156.011	396.560	1019.400	-62.284	790.755	865.516	-452.090
200	311.865	549.907	746.259	-39.270	771.746	947.895	-247.560
250	401.681	629.085	714.866	-21.445	762.967	992.949	-207.461
298.15	488.812	707.308	707.308	0.000	755.233	1037.966	-181.844
300	492.113	710.342	707.317	0.907	754.949	1039.718	-181.027
350	578.770	792.779	713.630	27.702	747.907	1087.754	-162.335
400	658.932	875.377	728.689	58.675	741.877	1136.714	-148.437
450	731.413	957.251	749.547	93.467	736.733	1186.384	-137.709
500	796.103	1037.727	774.355	131.686	732.347	1236.615	-129.186
600	904.407	1192.843	831.295	216.929	725.407	1338.161	-116.495
700	989.933	1338.933	893.491	311.809	720.595	1440.704	-107.504
800	1058.471	1475.756	957.817	414.351	717.656	1543.784	-100.797
900	1114.301	1603.758	1022.556	523.081	716.342	1647.123	-95.595
1000	1160.413	1723.622	1086.734	636.888	716.431	1750.550	-91.437
1100	1198.915	1836.081	1149.798	754.911	717.653	1853.925	-88.034
1200	1231.344	1941.830	1211.439	876.469	719.815	1957.120	-85.189
1300	1258.856	2041.506	1271.494	1001.016	722.669	2060.122	-82.775
1400	1282.345	2135.679	1329.889	1128.107	726.035	2162.888	-80.697
1500	1302.514	2224.857	1386.607	1257.375	729.803	2265.402	-78.887
1600	1319.926	2309.489	1441.665	1388.517	733.795	2367.643	-77.294
1700	1335.034	2389.973	1495.100	1521.283	737.911	2469.597	-75.880
1800	1348.207	2466.663	1546.963	1655.460	742.047	2571.397	-74.618
1900	1359.745	2539.872	1597.309	1790.870	746.164	2672.894	-73.481
2000	1369.897	2609.882	1646.200	1927.363	750.184	2774.213	-72.454
2100	1378.866	2676.941	1693.698	2064.810	754.004	2875.315	-71.518
2200	1386.823	2741.273	1739.863	2203.102	757.621	2976.244	-70.664
2300	1393.908	2803.079	1784.755	2342.146	761.029	3077.012	-69.880
2400	1400.240	2862.539	1828.431	2481.859	764.131	3177.571	-69.157
2500	1405.918	2919.817	1870.948	2622.172	766.944	3278.164	-68.492
2600	1411.028	2975.059	1912.358	2763.023	769.418	3378.489	-67.873
2700	1415.640	3028.400	1952.711	2904.361	771.559	3478.825	-67.301
2800	1419.816	3079.960	1992.054	3046.137	773.333	3579.120	-66.768
2900	1423.607	3129.851	2030.433	3188.311	774.697	3679.283	-66.270
3000	1427.059	3178.172	2067.890	3330.847	775.714	3779.442	-65.805
3100	1430.209	3225.017	2104.465	3473.713	776.275	3879.468	-65.367
3200	1433.091	3270.471	2140.196	3616.880	776.441	3979.584	-64.959
3300	1435.735	3314.610	2175.119	3760.323	776.184	4079.756	-64.576
3400	1438.165	3357.508	2209.267	3904.020	775.467	4179.822	-64.214
3500	1440.403	3399.230	2242.672	4047.950	774.295	4279.890	-63.873
3600	1442.469	3439.836	2275.366	4192.095	772.701	4380.120	-63.553
3700	1444.380	3479.385	2307.374	4336.438	770.641	4480.424	-63.251
3800	1446.150	3517.928	2338.726	4480.966	768.078	4580.706	-62.965
3900	1447.793	3555.514	2369.446	4625.664	765.069	4680.990	-62.694
4000	1449.321	3592.188	2399.558	4770.521	761.592	4781.551	-62.439
4100	1450.744	3627.993	2429.085	4915.525	757.597	4882.101	-62.197
4200	1452.071	3662.969	2458.048	5060.667	753.123	4982.742	-61.968
4300	1453.311	3697.152	2486.469	5205.936	748.151	5083.370	-61.749
4400	1454.471	3730.576	2514.365	5351.326	742.694	5184.248	-61.544
4500	1455.557	3763.274	2541.757	5496.828	736.771	5285.333	-61.349
4600	1456.577	3795.277	2568.661	5642.435	730.310	5386.567	-61.165
4700	1457.534	3826.613	2595.093	5788.141	723.332	5487.788	-60.989
4800	1458.434	3857.309	2621.071	5933.940	715.902	5589.311	-60.823
4900	1459.282	3887.389	2646.608	6079.826	707.916	5690.804	-60.663
5000	1460.081	3916.879	2671.720	6225.795	699.506	5792.727	-60.515

3.662. Tetrabenzo[*a,c,l,n*]pentacene



Formula: C₃₈H₂₂
Mass: 478.581 g/mol
CAS Number: 216-07-9
Point Group: D_{2h}

Length: 19.02 Å
Width: 11.66 Å
Breadth: 3.885 Å
L/B Ratio: 1.631

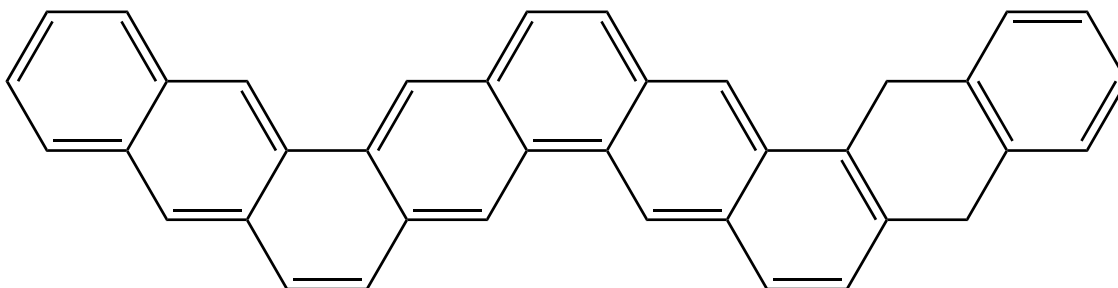
Cartesian coordinates:

C	-7.3595	2.8249	0.0000	C	1.2125	0.7119	0.0000	H	-4.0015	3.3870	0.0000
C	-7.3506	1.4412	0.0000	C	1.2132	-0.7106	0.0000	H	-6.1586	4.6219	0.0000
C	-4.9552	2.8371	0.0000	C	2.4630	-1.3956	0.0000	H	-8.2985	-0.8913	0.0000
C	-6.1545	3.5271	0.0000	C	2.4616	1.3981	0.0000	H	-8.3066	-3.3765	0.0000
C	-4.9288	1.4337	0.0000	C	3.6552	0.7209	0.0000	H	-6.1539	-4.6280	0.0000
C	-6.1427	0.7267	0.0000	C	3.6559	-0.7172	0.0000	H	-3.9981	-3.3910	0.0000
C	-4.9273	-1.4386	0.0000	C	4.9273	1.4387	0.0000	H	-2.4567	-2.5002	0.0000
C	-6.1420	-0.7328	0.0000	C	6.1420	0.7328	0.0000	H	-2.4592	2.4977	0.0000
C	-7.3492	-1.4485	0.0000	C	7.3492	1.4486	0.0000	H	0.0012	-2.5028	0.0000
C	-7.3567	-2.8322	0.0000	C	7.3567	2.8323	0.0000	H	-0.0013	2.5028	0.0000
C	-6.1510	-3.5333	0.0000	C	6.1510	3.5333	0.0000	H	2.4592	-2.4977	0.0000
C	-4.9523	-2.8420	0.0000	C	4.9523	2.8420	0.0000	H	2.4567	2.5002	0.0000
C	-3.6559	0.7172	0.0000	C	6.1427	-0.7267	0.0000	H	8.2985	0.8914	0.0000
C	-3.6552	-0.7209	0.0000	C	4.9287	-1.4337	0.0000	H	8.3066	3.3765	0.0000
C	-2.4616	-1.3981	0.0000	C	4.9552	-2.8371	0.0000	H	6.1539	4.6280	0.0000
C	-2.4630	1.3956	0.0000	C	6.1545	-3.5271	0.0000	H	3.9982	3.3910	0.0000
C	-1.2132	0.7107	0.0000	C	7.3595	-2.8249	0.0000	H	4.0015	-3.3870	0.0000
C	-1.2125	-0.7119	0.0000	C	7.3506	-1.4412	0.0000	H	6.1585	-4.6219	0.0000
C	0.0007	-1.4059	0.0000	H	-8.3100	3.3682	0.0000	H	8.3099	-3.3682	0.0000
C	-0.0007	1.4059	0.0000	H	-8.2993	0.8830	0.0000	H	8.2994	-0.8831	0.0000

Table 3.662: Table of thermodynamic data as a function of temperature for Tetra-benzo[*a,c,l,n*]pentacene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	<i>C</i> _{<i>p</i>} ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) - <i>H</i> ^o (<i>T</i> _{<i>r</i>})	$\Delta_f H^o$	$\Delta_f G^o$	log <i>K</i> _{<i>f</i>}
0	0.0	0.0	∞	-72.415	650.937	650.937	∞
100	161.785	420.213	1045.000	-62.479	686.264	758.660	-396.275
200	312.511	576.014	771.719	-39.141	667.580	838.506	-218.991
250	400.227	655.099	740.454	-21.339	658.778	882.256	-184.333
298.15	485.933	732.936	732.936	0.000	650.937	926.029	-162.233
300	489.190	735.952	732.945	0.902	650.648	927.734	-161.529
350	574.926	817.863	739.219	27.526	643.434	974.502	-145.433
400	654.583	899.911	754.180	58.292	637.198	1022.221	-133.486
450	726.848	981.257	774.902	92.860	631.831	1070.678	-124.279
500	791.512	1061.251	799.551	130.850	627.215	1119.721	-116.974
600	900.055	1215.546	856.141	215.643	619.825	1218.958	-106.118
700	985.959	1360.993	917.983	310.107	614.597	1319.264	-98.443
800	1054.885	1497.311	981.973	412.271	611.279	1420.163	-92.725
900	1111.073	1624.911	1046.399	520.661	609.625	1521.368	-88.296
1000	1157.505	1744.453	1110.292	634.161	609.408	1622.697	-84.759
1100	1196.290	1856.648	1173.095	751.908	610.353	1724.002	-81.864
1200	1228.969	1962.179	1234.499	873.216	612.266	1825.152	-79.445
1300	1256.702	2061.674	1294.338	997.537	614.893	1926.128	-77.391
1400	1280.386	2155.695	1352.537	1124.422	618.054	2026.885	-75.622
1500	1300.728	2244.744	1409.075	1253.503	621.635	2127.404	-74.081
1600	1318.294	2329.265	1463.969	1384.475	625.457	2227.662	-72.724
1700	1333.539	2409.655	1517.252	1517.084	629.416	2327.643	-71.518
1800	1346.834	2486.263	1568.975	1651.118	633.409	2427.479	-70.442
1900	1358.482	2559.401	1619.192	1786.396	637.394	2527.020	-69.471
2000	1368.731	2629.348	1667.964	1922.768	641.293	2626.389	-68.593
2100	1377.787	2696.352	1715.351	2060.103	645.000	2725.547	-67.793
2200	1385.822	2760.636	1761.413	2198.291	648.514	2824.538	-67.062
2300	1392.978	2822.399	1806.209	2337.238	651.825	2923.372	-66.390
2400	1399.374	2881.821	1849.796	2476.861	654.838	3022.000	-65.771
2500	1405.111	2939.065	1892.229	2617.091	657.567	3120.667	-65.201
2600	1410.273	2994.277	1933.560	2757.864	659.963	3219.068	-64.671
2700	1414.933	3047.590	1973.839	2899.129	662.031	3317.484	-64.179
2800	1419.153	3099.125	2013.112	3040.836	663.736	3415.861	-63.722
2900	1422.984	3148.993	2051.425	3182.946	665.036	3514.109	-63.295
3000	1426.472	3197.294	2088.820	3325.422	665.992	3612.355	-62.895
3100	1429.656	3244.121	2125.336	3468.231	666.497	3710.469	-62.520
3200	1432.569	3289.557	2161.012	3611.344	666.609	3808.676	-62.169
3300	1435.241	3333.681	2195.882	3754.736	666.301	3906.941	-61.840
3400	1437.697	3376.564	2229.980	3898.385	665.536	4005.100	-61.530
3500	1439.960	3418.273	2263.338	4042.269	664.319	4103.263	-61.237
3600	1442.048	3458.867	2295.986	4186.371	662.682	4201.589	-60.962
3700	1443.980	3498.404	2327.952	4330.674	660.580	4299.991	-60.704
3800	1445.769	3536.937	2359.263	4475.162	657.978	4398.371	-60.459
3900	1447.431	3574.513	2389.943	4619.823	654.932	4496.755	-60.226
4000	1448.975	3611.179	2420.018	4764.645	651.419	4595.416	-60.009
4100	1450.414	3646.976	2449.509	4909.615	647.390	4694.068	-59.802
4200	1451.756	3681.943	2478.438	5054.724	642.885	4792.811	-59.606
4300	1453.009	3716.119	2506.825	5199.963	637.882	4891.542	-59.419
4400	1454.182	3749.536	2534.690	5345.323	632.395	4990.523	-59.244
4500	1455.280	3782.228	2562.051	5490.797	626.443	5089.713	-59.079
4600	1456.311	3814.225	2588.926	5636.377	619.956	5189.052	-58.922
4700	1457.279	3845.555	2615.330	5782.057	612.952	5288.378	-58.773
4800	1458.189	3876.246	2641.281	5927.831	605.496	5388.007	-58.632
4900	1459.046	3906.321	2666.792	6073.693	597.487	5487.606	-58.497
5000	1459.854	3935.806	2691.879	6219.638	589.053	5587.637	-58.372

3.663. Dinaphtho[2,3-*c*:2',3'-*m*]pentaphene



Formula: C₃₈H₂₂
Mass: 478.581 g/mol
CAS Number: 133979-16-5
Point Group: C_{2v}

Length: 24.45 Å
Width: 9.180 Å
Breadth: 3.884 Å
L/B Ratio: 2.663

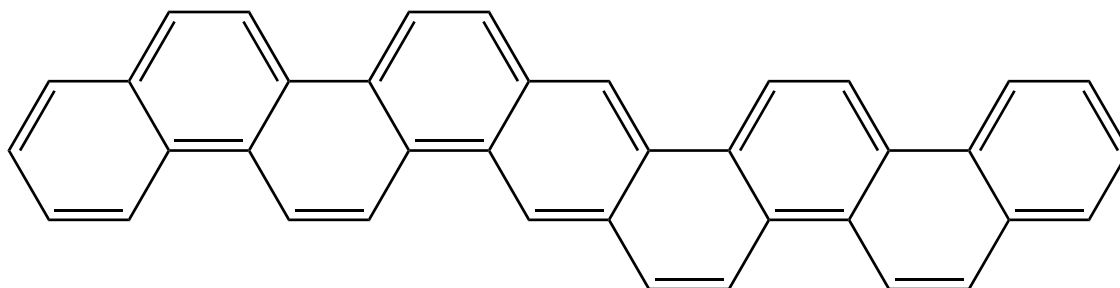
Cartesian coordinates:

C	-9.2402	2.1960	0.0000	C	1.4172	1.0204	0.0000	H	-9.7644	-1.1834	0.0000
C	-9.9303	0.9555	0.0000	C	0.7259	-0.2113	0.0000	H	-7.3352	3.1826	0.0000
C	-9.2397	-0.2213	0.0000	C	1.4555	-1.4044	0.0000	H	-7.6151	-2.3779	0.0000
C	-7.8761	2.2296	0.0000	C	2.8155	1.0307	0.0000	H	-5.1757	1.9855	0.0000
C	-7.1256	1.0163	0.0000	C	3.5416	-0.1588	0.0000	H	-5.5021	-3.5768	0.0000
C	-7.8130	-0.2196	0.0000	C	2.8486	-1.3924	0.0000	H	-3.0238	-3.5697	0.0000
C	-7.0778	-1.4214	0.0000	C	3.5927	-2.6313	0.0000	H	-0.9057	-2.3603	0.0000
C	-5.7174	1.0258	0.0000	C	4.9404	-2.6344	0.0000	H	-3.3628	1.9868	0.0000
C	-4.9979	-0.1576	0.0000	C	4.9979	-0.1561	0.0000	H	1.2402	3.1954	0.0000
C	-5.6929	-1.4013	0.0000	C	5.6934	-1.3997	0.0000	H	-1.2411	3.1951	0.0000
C	-4.9396	-2.6358	0.0000	C	7.0782	-1.4194	0.0000	H	0.9063	-2.3600	0.0000
C	-3.5920	-2.6323	0.0000	C	5.7171	1.0274	0.0000	H	3.3622	1.9877	0.0000
C	-3.5416	-0.1598	0.0000	C	7.1253	1.0184	0.0000	H	3.0247	-3.5689	0.0000
C	-2.8482	-1.3932	0.0000	C	7.8131	-0.2173	0.0000	H	5.5032	-3.5753	0.0000
C	-1.4551	-1.4048	0.0000	C	9.2398	-0.2186	0.0000	H	7.6159	-2.3757	0.0000
C	-2.8158	1.0299	0.0000	C	9.9301	0.9585	0.0000	H	5.1751	1.9869	0.0000
C	-1.4176	1.0200	0.0000	C	9.2396	2.1987	0.0000	H	9.7649	-1.1805	0.0000
C	-0.7258	-0.2114	0.0000	C	7.8754	2.2319	0.0000	H	11.0250	0.9633	0.0000
C	0.6750	2.2562	0.0000	H	-9.8213	3.1240	0.0000	H	9.8204	3.1269	0.0000
C	-0.6757	2.2560	0.0000	H	-11.0252	0.9600	0.0000	H	7.3342	3.1847	0.0000

Table 3.663: Table of thermodynamic data as a function of temperature for Dinaphtho[2,3-c:2',3'-m]pentaphene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			
	C _p ^o	S ^o	$-\frac{G^o-H^o(298\text{ K})}{T}$	H ^o (T) – H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _f
0	0.0	0.0	∞	-71.628	622.074	622.074	∞
100	157.229	412.818	1034.800	-62.198	657.682	730.817	-381.732
200	311.367	566.591	762.258	-39.133	638.724	811.536	-211.947
250	400.236	645.552	730.983	-21.358	629.896	855.761	-178.798
298.15	486.655	723.457	723.457	0.000	622.074	899.992	-157.672
300	489.933	726.477	723.466	0.903	621.786	901.714	-156.999
350	576.061	808.536	729.750	27.575	614.621	948.953	-141.621
400	655.887	890.749	744.740	58.404	608.446	997.135	-130.210
450	728.197	972.252	765.501	93.038	603.146	1046.046	-121.419
500	792.848	1052.387	790.196	131.095	598.597	1095.535	-114.447
600	901.319	1206.920	846.889	216.019	591.337	1195.646	-104.088
700	987.168	1352.557	908.834	310.606	586.232	1296.805	-96.767
800	1056.062	1489.034	972.923	412.889	583.034	1398.540	-91.313
900	1112.228	1616.772	1037.444	521.395	581.497	1500.566	-87.089
1000	1158.634	1736.434	1101.424	635.010	581.394	1602.702	-83.715
1100	1197.387	1848.735	1164.310	752.868	582.450	1704.804	-80.953
1200	1230.026	1954.360	1225.790	874.284	584.471	1806.740	-78.644
1300	1257.712	2053.938	1285.701	998.708	587.202	1908.493	-76.683
1400	1281.346	2148.032	1343.967	1125.692	590.461	2010.021	-74.993
1500	1301.637	2237.145	1400.568	1254.866	594.136	2111.303	-73.521
1600	1319.151	2321.724	1455.520	1385.927	598.045	2212.318	-72.223
1700	1334.345	2402.163	1508.858	1518.619	602.088	2313.051	-71.070
1800	1347.592	2478.816	1560.632	1652.731	606.160	2413.633	-70.040
1900	1359.193	2551.994	1610.898	1788.083	610.217	2513.917	-69.111
2000	1369.398	2621.976	1659.715	1924.523	614.186	2614.025	-68.270
2100	1378.414	2689.012	1707.144	2061.923	617.957	2713.919	-67.504
2200	1386.411	2753.324	1753.246	2200.172	621.531	2813.642	-66.803
2300	1393.531	2815.113	1798.080	2339.176	624.900	2913.205	-66.160
2400	1399.894	2874.558	1841.703	2478.853	627.966	3012.561	-65.565
2500	1405.600	2931.822	1884.169	2619.132	630.746	3111.954	-65.019
2600	1410.734	2987.052	1925.532	2759.954	633.189	3211.078	-64.510
2700	1415.368	3040.382	1965.841	2901.263	635.302	3310.216	-64.039
2800	1419.563	3091.933	2005.143	3043.013	637.049	3409.312	-63.600
2900	1423.372	3141.815	2043.483	3185.162	638.389	3508.279	-63.190
3000	1426.839	3190.129	2080.904	3327.675	639.383	3607.242	-62.806
3100	1430.003	3236.967	2117.444	3470.520	639.924	3706.072	-62.446
3200	1432.898	3282.414	2153.143	3613.667	640.069	3804.994	-62.109
3300	1435.554	3326.548	2188.035	3757.092	639.793	3903.972	-61.793
3400	1437.994	3369.440	2222.155	3900.771	639.058	4002.844	-61.495
3500	1440.242	3411.157	2255.533	4044.684	637.871	4101.719	-61.214
3600	1442.317	3451.759	2288.200	4188.813	636.261	4200.757	-60.950
3700	1444.236	3491.304	2320.184	4333.142	634.186	4299.869	-60.702
3800	1446.014	3529.843	2351.512	4477.656	631.609	4398.959	-60.467
3900	1447.664	3567.426	2382.210	4622.341	628.587	4498.051	-60.243
4000	1449.198	3604.097	2412.301	4767.185	625.097	4597.422	-60.035
4100	1450.627	3639.899	2441.807	4912.177	621.090	4696.781	-59.836
4200	1451.960	3674.872	2470.751	5057.307	616.605	4796.232	-59.649
4300	1453.205	3709.052	2499.153	5202.566	611.622	4895.669	-59.469
4400	1454.370	3742.474	2527.032	5347.945	606.154	4995.357	-59.301
4500	1455.461	3775.170	2554.406	5493.438	600.221	5095.253	-59.143
4600	1456.484	3807.171	2581.294	5639.035	593.751	5195.298	-58.993
4700	1457.445	3838.505	2607.711	5784.732	586.764	5295.329	-58.850
4800	1458.349	3869.198	2633.673	5930.522	579.325	5395.662	-58.716
4900	1459.200	3899.277	2659.196	6076.400	571.331	5495.967	-58.587
5000	1460.002	3928.765	2684.293	6222.361	562.913	5596.701	-58.467

3.664. Chryseno[2,1-*b*]picene



Formula: C₃₈H₂₂
Mass: 478.581 g/mol
CAS Number: 119000-37-2
Point Group: C_{2h}

Length: 24.31 Å
Width: 8.909 Å
Breadth: 3.885 Å
L/B Ratio: 2.728

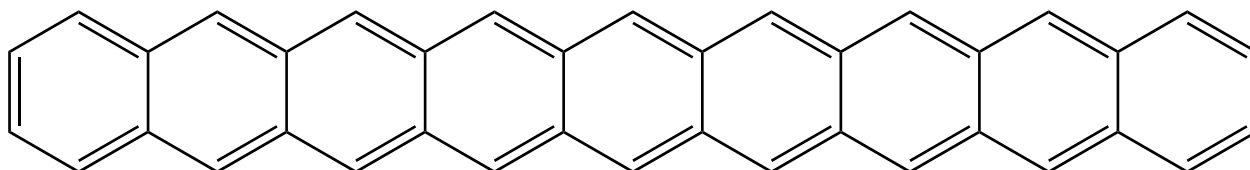
Cartesian coordinates:

C	9.1407	-1.8023	0.0000	C	-0.7913	-1.1573	0.0000	H	9.8794	1.5268	0.0000
C	9.9078	-0.6233	0.0000	C	-1.4064	0.1189	0.0000	H	7.1565	-2.6508	0.0000
C	9.2884	0.6039	0.0000	C	-2.9640	-2.2382	0.0000	H	7.8416	2.8694	0.0000
C	7.7680	-1.7355	0.0000	C	-1.6150	-2.3356	0.0000	H	5.3627	3.0239	0.0000
C	7.1072	-0.4856	0.0000	C	-3.6231	-0.9599	0.0000	H	2.8723	-2.3757	0.0000
C	7.8776	0.6906	0.0000	C	-2.8527	0.2068	0.0000	H	5.3656	-2.5383	0.0000
C	7.2226	1.9649	0.0000	C	-3.4990	1.4706	0.0000	H	3.5964	3.1392	0.0000
C	5.8693	2.0467	0.0000	C	-4.8613	1.5597	0.0000	H	1.1202	3.3137	0.0000
C	5.6664	-0.3904	0.0000	C	-5.0515	-0.8686	0.0000	H	-1.0813	2.2515	0.0000
C	5.0515	0.8686	0.0000	C	-5.6665	0.3904	0.0000	H	1.0814	-2.2514	0.0000
C	3.4990	-1.4706	0.0000	C	-7.2225	-1.9649	0.0000	H	-3.5963	-3.1392	0.0000
C	4.8613	-1.5597	0.0000	C	-5.8693	-2.0468	0.0000	H	-1.1201	-3.3137	0.0000
C	2.8527	-0.2068	0.0000	C	-7.8776	-0.6907	0.0000	H	-2.8723	2.3758	0.0000
C	3.6231	0.9599	0.0000	C	-7.1073	0.4856	0.0000	H	-5.3657	2.5383	0.0000
C	2.9641	2.2382	0.0000	C	-7.7680	1.7355	0.0000	H	-7.8415	-2.8694	0.0000
C	1.6150	2.3357	0.0000	C	-9.1407	1.8022	0.0000	H	-5.3627	-3.0239	0.0000
C	1.4065	-0.1188	0.0000	C	-9.9078	0.6232	0.0000	H	-7.1566	2.6507	0.0000
C	0.7913	1.1574	0.0000	C	-9.2884	-0.6040	0.0000	H	-9.6467	2.7732	0.0000
C	-0.6009	1.2597	0.0000	H	9.6466	-2.7733	0.0000	H	-11.0005	0.6924	0.0000
C	0.6009	-1.2596	0.0000	H	11.0005	-0.6926	0.0000	H	-9.8793	-1.5269	0.0000

Table 3.664: Table of thermodynamic data as a function of temperature for Chryseno[2,1-*b*]picene.

<i>T</i> [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log <i>K_f</i>
	<i>C_p</i> ^o	<i>S</i> ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	<i>H</i> ^o (<i>T</i>) – <i>H</i> ^o (<i>T_r</i>)	$\Delta_f H^o$	$\Delta_f G^o$	
0	0.0	0.0	∞	-71.894	615.545	615.545	∞
100	159.416	420.922	1042.913	-62.199	651.152	723.477	-377.898
200	311.209	575.383	770.626	-39.049	632.281	803.334	-209.805
250	399.334	654.226	739.427	-21.300	623.425	847.122	-176.993
298.15	485.191	731.922	731.922	0.000	615.545	890.940	-156.086
300	488.450	734.933	731.931	0.901	615.255	892.647	-155.420
350	574.190	816.731	738.195	27.488	608.005	939.469	-140.205
400	653.799	898.679	753.137	58.217	601.731	987.248	-128.919
450	726.014	979.929	773.832	92.744	596.323	1035.768	-120.226
500	790.646	1059.833	798.450	130.691	591.665	1084.880	-113.334
600	899.188	1213.969	854.974	215.397	584.188	1184.267	-103.097
700	985.148	1359.286	916.748	309.777	578.875	1284.737	-95.866
800	1054.154	1495.501	980.672	411.863	575.481	1385.813	-90.482
900	1110.425	1623.020	1045.037	520.185	573.758	1487.203	-86.313
1000	1156.935	1742.498	1108.874	633.624	573.480	1588.724	-82.985
1100	1195.790	1854.642	1171.626	751.317	574.371	1690.227	-80.261
1200	1228.529	1960.132	1232.983	872.579	576.237	1791.580	-77.984
1300	1256.313	2059.594	1292.780	996.858	578.823	1892.762	-76.051
1400	1280.041	2153.588	1350.941	1123.706	581.948	1993.729	-74.385
1500	1300.421	2242.614	1407.444	1252.755	585.496	2094.460	-72.934
1600	1318.019	2327.117	1462.305	1383.698	589.288	2194.932	-71.656
1700	1333.292	2407.490	1515.560	1516.281	593.221	2295.129	-70.519
1800	1346.611	2484.084	1567.256	1650.291	597.191	2395.182	-69.505
1900	1358.279	2557.211	1617.449	1785.548	601.155	2494.941	-68.589
2000	1368.546	2627.148	1666.198	1921.900	605.035	2594.530	-67.761
2100	1377.619	2694.144	1713.564	2059.218	608.724	2693.908	-67.006
2200	1385.668	2758.420	1759.607	2197.390	612.221	2793.120	-66.316
2300	1392.836	2820.177	1804.385	2336.322	615.518	2892.176	-65.682
2400	1399.243	2879.593	1847.955	2475.932	618.517	2991.027	-65.097
2500	1404.990	2936.832	1890.372	2616.148	621.234	3089.917	-64.559
2600	1410.161	2992.039	1931.689	2756.910	623.618	3188.541	-64.057
2700	1414.829	3045.348	1971.954	2898.164	625.675	3287.181	-63.593
2800	1419.055	3096.880	2011.215	3039.861	627.370	3385.783	-63.161
2900	1422.893	3146.744	2049.516	3181.962	628.660	3484.255	-62.757
3000	1426.386	3195.042	2086.899	3324.429	629.608	3582.726	-62.380
3100	1429.576	3241.866	2123.405	3467.229	630.105	3681.066	-62.024
3200	1432.494	3287.300	2159.070	3610.335	630.208	3779.498	-61.693
3300	1435.170	3331.422	2193.931	3753.720	629.893	3877.989	-61.382
3400	1437.630	3374.303	2228.020	3897.361	629.121	3976.374	-61.088
3500	1439.896	3416.009	2261.369	4041.239	627.898	4074.763	-60.811
3600	1441.988	3456.602	2294.009	4185.335	626.254	4173.316	-60.552
3700	1443.923	3496.138	2325.967	4329.632	624.147	4271.945	-60.308
3800	1445.715	3534.669	2357.270	4474.115	621.539	4370.552	-60.076
3900	1447.379	3572.244	2387.944	4618.770	618.488	4469.162	-59.856
4000	1448.926	3608.908	2418.011	4763.587	614.970	4568.050	-59.651
4100	1450.367	3644.704	2447.496	4908.552	610.937	4666.929	-59.456
4200	1451.711	3679.670	2476.419	5053.657	606.426	4765.900	-59.271
4300	1452.967	3713.845	2504.800	5198.892	601.419	4864.858	-59.095
4400	1454.141	3747.261	2532.660	5344.248	595.928	4964.067	-58.930
4500	1455.242	3779.952	2560.015	5489.717	589.973	5063.484	-58.774
4600	1456.274	3811.948	2586.885	5635.294	583.481	5163.051	-58.627
4700	1457.243	3843.278	2613.284	5780.970	576.473	5262.604	-58.486
4800	1458.155	3873.967	2639.230	5926.740	569.015	5362.461	-58.354
4900	1459.013	3904.042	2664.737	6072.599	561.002	5462.288	-58.228
5000	1459.823	3933.527	2689.818	6218.541	552.565	5562.546	-58.110

3.665. Nonacene



Formula: $C_{38}H_{22}$
Mass: 478.581 g/mol
CAS Number: 258-36-6
Point Group: D_{2h}

Length: 26.27 Å
Width: 7.442 Å
Breadth: 3.882 Å
L/B Ratio: 3.530

Cartesian coordinates:

C	-10.9676	0.7201	0.0000	C	1.2182	0.7165	0.0000	H	-9.7977	-2.5050	0.0000
C	-10.9677	-0.7181	0.0000	C	1.2181	-0.7167	0.0000	H	-9.7972	2.5068	0.0000
C	-9.8072	-1.4091	0.0000	C	2.4509	-1.4071	0.0000	H	-7.3440	-2.5070	0.0000
C	-9.8069	1.4108	0.0000	C	2.4512	1.4066	0.0000	H	-7.3435	2.5083	0.0000
C	-8.5334	0.7238	0.0000	C	3.6551	0.7180	0.0000	H	-4.8953	-2.5052	0.0000
C	-8.5335	-0.7223	0.0000	C	3.6550	-0.7187	0.0000	H	-4.8948	2.5061	0.0000
C	-7.3522	-1.4099	0.0000	C	4.9015	-1.4089	0.0000	H	-2.4475	-2.5039	0.0000
C	-7.3519	1.4112	0.0000	C	4.9017	1.4080	0.0000	H	-2.4470	2.5043	0.0000
C	-6.0937	0.7213	0.0000	C	6.0939	0.7202	0.0000	H	-0.0002	-2.5034	0.0000
C	-6.0938	-0.7203	0.0000	C	6.0938	-0.7212	0.0000	H	0.0002	2.5034	0.0000
C	-4.9019	-1.4081	0.0000	C	7.3518	-1.4111	0.0000	H	2.4470	-2.5043	0.0000
C	-4.9016	1.4089	0.0000	C	7.3521	1.4099	0.0000	H	2.4475	2.5038	0.0000
C	-3.6548	0.7188	0.0000	C	8.5336	0.7222	0.0000	H	4.8948	-2.5060	0.0000
C	-3.6549	-0.7181	0.0000	C	8.5334	-0.7237	0.0000	H	4.8952	2.5052	0.0000
C	-2.4514	-1.4067	0.0000	C	9.8069	-1.4108	0.0000	H	7.3435	-2.5082	0.0000
C	-2.4511	1.4071	0.0000	C	10.9676	-0.7200	0.0000	H	7.3439	2.5070	0.0000
C	-1.2178	0.7167	0.0000	C	10.9677	0.7181	0.0000	H	9.7972	-2.5067	0.0000
C	-1.2179	-0.7166	0.0000	C	9.8071	1.4091	0.0000	H	11.9328	-1.2368	0.0000
C	-0.0002	-1.4062	0.0000	H	-11.9328	1.2368	0.0000	H	11.9330	1.2348	0.0000
C	-0.0000	1.4062	0.0000	H	-11.9331	-1.2347	0.0000	H	9.7976	2.5050	0.0000

Table 3.665: Table of thermodynamic data as a function of temperature for Nonacene.

T [K]	[J mol ⁻¹ K ⁻¹]			[kJ mol ⁻¹]			log K _f
	C _p ^o	S ^o	$-\frac{G^o - H^o(298\text{ K})}{T}$	H ^o (T) - H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	
0	0.0	0.0	∞	-71.884	784.472	784.472	∞
100	156.767	403.210	1028.918	-62.571	819.707	893.803	-466.865
200	313.443	557.364	754.545	-39.436	800.820	975.476	-254.763
250	403.431	636.919	723.025	-21.527	792.125	1020.149	-213.144
298.15	490.389	715.440	715.440	0.000	784.472	1064.781	-186.541
300	493.678	718.483	715.449	0.910	784.191	1066.518	-185.693
350	579.929	801.133	721.779	27.774	777.218	1114.141	-166.273
400	659.642	883.856	736.873	58.793	771.234	1162.680	-151.827
450	731.733	965.790	757.767	93.610	766.116	1211.924	-140.674
500	796.130	1046.284	782.608	131.838	761.738	1261.727	-131.809
600	904.112	1201.371	839.597	217.065	754.781	1362.419	-118.607
700	989.554	1347.407	901.821	311.910	749.935	1464.112	-109.251
800	1058.122	1484.181	966.163	414.415	746.959	1566.346	-102.270
900	1114.026	1612.146	1030.908	523.114	745.614	1668.846	-96.855
1000	1160.219	1731.986	1095.089	636.897	745.679	1771.435	-92.528
1100	1198.794	1844.429	1158.153	754.904	746.885	1873.975	-88.986
1200	1231.282	1950.170	1219.793	876.453	749.038	1976.335	-86.026
1300	1258.840	2049.843	1279.846	1000.997	751.888	2078.503	-83.514
1400	1282.364	2144.017	1338.240	1128.087	755.255	2180.436	-81.351
1500	1302.558	2233.197	1394.958	1257.358	759.026	2282.116	-79.469
1600	1319.988	2317.832	1450.015	1388.507	763.024	2383.523	-77.812
1700	1335.109	2398.320	1503.450	1521.279	767.146	2484.642	-76.342
1800	1348.290	2475.014	1555.312	1655.464	771.291	2585.607	-75.031
1900	1359.834	2548.229	1605.659	1790.883	775.416	2686.269	-73.849
2000	1369.988	2618.243	1654.551	1927.385	779.445	2786.752	-72.781
2100	1378.958	2685.306	1702.049	2064.841	783.274	2887.018	-71.809
2200	1386.914	2749.643	1748.214	2203.142	786.900	2987.110	-70.922
2300	1393.998	2811.453	1793.107	2342.195	790.318	3087.041	-70.107
2400	1400.328	2870.917	1836.785	2481.917	793.429	3186.762	-69.357
2500	1406.005	2928.198	1879.303	2622.239	796.251	3286.517	-68.667
2600	1411.112	2983.444	1920.714	2763.099	798.733	3386.003	-68.024
2700	1415.721	3036.788	1961.068	2904.444	800.882	3485.501	-67.430
2800	1419.894	3088.351	2000.412	3046.229	802.664	3584.956	-66.877
2900	1423.683	3138.244	2038.792	3188.411	804.035	3684.280	-66.360
3000	1427.131	3186.568	2076.250	3330.954	805.060	3783.600	-65.877
3100	1430.279	3233.416	2112.826	3473.827	805.629	3882.786	-65.423
3200	1433.159	3278.871	2148.559	3617.001	805.801	3982.062	-64.999
3300	1435.800	3323.013	2183.482	3760.450	805.550	4081.395	-64.602
3400	1438.227	3365.912	2217.632	3904.153	804.839	4180.620	-64.226
3500	1440.463	3407.636	2251.039	4048.089	803.674	4279.848	-63.872
3600	1442.526	3448.244	2283.733	4192.240	802.086	4379.237	-63.540
3700	1444.435	3487.794	2315.743	4336.590	800.031	4478.700	-63.227
3800	1446.203	3526.339	2347.096	4481.123	797.473	4578.141	-62.930
3900	1447.844	3563.926	2377.817	4625.826	794.470	4677.584	-62.648
4000	1449.370	3600.602	2407.930	4770.688	790.997	4777.303	-62.384
4100	1450.791	3636.408	2437.458	4915.697	787.007	4877.012	-62.133
4200	1452.116	3671.385	2466.422	5060.843	782.539	4976.812	-61.894
4300	1453.355	3705.568	2494.843	5206.117	777.571	5076.598	-61.667
4400	1454.513	3738.994	2522.741	5351.511	772.118	5176.634	-61.453
4500	1455.598	3771.693	2550.134	5497.017	766.199	5276.878	-61.251
4600	1456.616	3803.697	2577.038	5642.628	759.742	5377.270	-61.060
4700	1457.571	3835.033	2603.472	5788.338	752.768	5477.649	-60.876
4800	1458.470	3865.730	2629.450	5934.141	745.341	5578.329	-60.703
4900	1459.317	3895.811	2654.988	6080.030	737.359	5678.980	-60.537
5000	1460.114	3925.301	2680.101	6226.002	728.952	5780.061	-60.383

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 1*H*-Indeno[2,1-*a*]anthracene, 208
 1*H*-Indeno[2,1-*a*]phenanthrene, 212
 4*H*-Benzo[*hi*]chrysene, 232
 4*H*-Dibenz[*a,kl*]anthracene, 228
 5*H*-Dibenzo[*c,mn*]phenanthrene, 220
 7*H*-Benzo[*hi*]chrysene, 234
 7*H*-Dibenz[*a,kl*]anthracene, 226
 7*H*-Dibenzo[*b,g*]fluorene, 198
 7*H*-Dibenzo[*c,g*]fluorene, 192
 7*H*-Indeno[1,2-*a*]phenanthrene, 204
 8*H*-Dibenzo[*b,mn*]phenanthrene, 222
 8*H*-Indeno[1,2-*a*]anthracene, 196
 8*H*-Indeno[2,1-*b*]phenanthrene, 200
 9*H*-Benzo[*a*]cyclopent[*i*]anthracene, 186
 9*H*-Indeno[2,1-*c*]phenanthrene, 188

$C_{22}H_{12}$
 Benzo[*def*]cyclopenta[*qr*]chrysene, 240
 Benzo[*ghi*]perylene, 262

Benzo[*l*]cyclopenta[*cd*]pyrene, 236
Cyclopenta[*cd*]perylene, 242
Dibenzo[*def,mno*]chrysene, 264
Indeno[1,2,3-*cd*]fluoranthene, 250
Indeno[1,2,3-*cd*]pyrene, 248
Indeno[1,7,6,5-*cdef*]chrysene, 244
Indeno[1,7-*ab*]pyrene, 246
Indeno[3,2,1,7-*defg*]chrysene, 258
Indeno[4,3,2,1-*cdef*]chrysene, 260
Indeno[5,6,7,1-*defg*]chrysene, 238
Indeno[6,7,1,2-*defg*]naphthacene, 254
Naphtho[4,5,6-*abc*]aceanthrylene, 256
Phenanthro[10,1,2,3-*cdef*]fluorene, 252

$C_{22}H_{14}$

Benzo[*a*]naphthacene, 280
Benzo[*b*]chrysene, 284
Benzo[*b*]triphenylene, 268
Benzo[*c*]chrysene, 274
Benzo[*g*]chrysene, 270
Dibenz[*a,h*]anthracene, 282
Dibenz[*a,j*]anthracene, 276
Dibenzo[*b,g*]phenanthrene, 272
Dibenzo[*c,g*]phenanthrene, 266
Pentacene, 288
Pentaphene, 278
Picene, 286

$C_{23}H_{12}$

1*H*-Benzo[*ghi*]cyclopenta[*pqr*]perylene, 290

$C_{23}H_{14}$

1*H*-Benzo[*b*]cyclopenta[*def*]triphenylene, 302
1*H*-Cyclopenta[*pqr*]picene, 318
1*H*-Cyclopenta[*rst*]pentaphene, 310
1*H*-Dibenz[*bc,j*]aceanthrylene, 314
1*H*-Dibenz[*bc,l*]aceanthrylene, 306
1*H*-Indeno[2,1,7-*gra*]naphthacene, 312
1*H*-Indeno[2,1-*a*]pyrene, 296
4*H*-Benzo[*b*]cyclopenta[*jkl*]triphenylene, 300
4*H*-Benzo[*b*]cyclopenta[*mno*]chrysene, 320
4*H*-Benzo[*c*]cyclopenta[*mno*]chrysene, 308
4*H*-Indeno[7,1,2-*ghi*]chrysene, 304
5*H*-Benzo[*b*]cyclopenta[*def*]chrysene, 316
6*H*-Cyclopenta[*ghi*]picene, 322
6*H*-Naphtho[1,2,3-*cd*]pyrene, 326
7*H*-Indeno[1,2-*a*]pyrene, 294
8*H*-Benzo[*g*]cyclopenta[*mno*]chrysene, 298

8*H*-Dibenzo[*b,fg*]pyrene, 324

9*H*-Indeno[1,2-*e*]pyrene, 292

C₂₄H₁₂

Acenaphtho[1,2,3-*cde*]pyrene, 338

Benz[*mno*]indeno[1,7,6,5-*cdef*]chrysene, 336

Benz[*mno*]indeno[5,6,7,1-*defg*]chrysene, 330

Benzo[*ghi*]cyclopenta[*cd*]perylene, 332

Coronene, 340

Dibenzo[*def,mno*]cyclopenta[*hi*]chrysene, 334

Indeno[5,6,7,1-*pqra*]perylene, 328

C₂₄H₁₄

as-Indaceno[2,3-*a*]phenanthrene, 372

Benz[5,6]indeno[2,1-*a*]phenalene, 380

Benz[*a*]indeno[1,2-*c*]fluorene, 374

Benz[*a*]indeno[2,1-*c*]naphthalene, 352

Benz[*a*]indeno[5,6-*g*]fluorene, 370

Benz[*b*]indeno[2,1-*h*]fluorene, 362

Benz[*c*]indeno[2,1-*a*]fluorene, 354

Benz[*de*]indeno[2,1-*b*]anthracene, 378

Benzo[*a*]cyclopenta[*de*]naphthacene, 410

Benzo[*a*]cyclopenta[*fg*]naphthacene, 420

Benzo[*a*]cyclopenta[*hi*]naphthacene, 436

Benzo[*a*]cyclopenta[*mn*]naphthacene, 418

Benzo[*a*]cyclopenta[*op*]naphthacene, 428

Benzo[*a*]perylene, 488

Benzo[*b*]cyclopenta[*hi*]chrysene, 430

Benzo[*b*]cyclopenta[*qr*]chrysene, 416

Benzo[*b*]perylene, 498

Benzo[*c*]cyclopenta[*hi*]chrysene, 402

Benzo[*c*]cyclopenta[*qr*]chrysene, 396

Benzo[*pqr*]picene, 506

Benzo[*rst*]pentaphene, 508

Cyclopent[*b*]indeno[4,5-*g*]phenanthrene, 342

Cyclopent[*b*]indeno[5,6-*g*]phenanthrene, 344

Cyclopent[*i*]indeno[5,6-*a*]anthracene, 350

Cyclopenta[*de*]pentacene, 442

Cyclopenta[*de*]pentaphene, 426

Cyclopenta[*de*]picene, 432

Cyclopenta[*fg*]pentacene, 440

Cyclopenta[*fg*]pentaphene, 406

Cyclopenta[*pq*]pentaphene, 408

Dibenz[*a,e*]aceanthrylene, 450

Dibenz[*a,e*]acephenanthrylene, 446

Dibenz[*a,j*]aceanthrylene, 466

Dibenz[*a,k*]acephenanthrylene, 388

Dibenz[*a,l*]aceanthrylene, 452
Dibenz[*e,j*]aceanthrylene, 398
Dibenz[*e,k*]acephenanthrylene, 478
Dibenz[*e,l*]aceanthrylene, 412
Dibenzo[*b,def*]chrysene, 510
Dibenzo[*c,i*]cyclopenta[*a*]fluorene, 346
Dibenzo[*c,mno*]chrysene, 500
Dibenzo[*de,mn*]naphthacene, 502
Dibenzo[*de,qr*]naphthacene, 492
Dibenzo[*def,p*]chrysene, 486
Dibenzo[*fg,op*]naphthacene, 496
Dibenzo[*j,l*]fluoranthene, 448
Dicyclopenta[*a,c*]naphthacene, 348
Fluoreno[2,1-*a*]fluorene, 364
Fluoreno[2,3-*a*]fluorene, 360
Fluoreno[3,2-*b*]fluorene, 368
Fluoreno[3,4-*b*]fluorene, 356
Fluoreno[4,3,2-*de*]anthracene, 376
Fluoreno[4,3-*c*]fluorene, 358
Indeno[1,2,3-*de*]naphthacene, 458
Indeno[1,2,3-*fg*]naphthacene, 454
Indeno[1,2,3-*hi*]chrysene, 468
Indeno[1,7-*ab*]chrysene, 434
Indeno[1,7-*ab*]triphenylene, 386
Indeno[7,1-*ab*]naphthacene, 438
Indeno[7,1-*ab*]triphenylene, 384
Indeno[7,1-*bc*]chrysene, 424
Naphth[1,2-*a*]aceanthrylene, 444
Naphth[1,2-*a*]acephenanthrylene, 382
Naphth[1,2-*e*]acephenanthrylene, 476
Naphth[1,2-*j*]aceanthrylene, 400
Naphth[1,2-*k*]acephenanthrylene, 422
Naphth[2,1-*a*]aceanthrylene, 464
Naphth[2,1-*e*]aceanthrylene, 392
Naphth[2,1-*e*]acephenanthrylene, 462
Naphth[2,1-*k*]acephenanthrylene, 414
Naphth[2,1-*l*]aceanthrylene, 394
Naphth[2,1-*l*]acephenanthrylene, 390
Naphth[2,3-*a*]aceanthrylene, 456
Naphth[2,3-*e*]acephenanthrylene, 472
Naphth[2,3-*l*]acephenanthrylene, 404
Naphtho[1,2,3,4-*def*]chrysene, 490
Naphtho[1,2-*j*]fluoranthene, 460
Naphtho[1,2-*k*]fluoranthene, 480
Naphtho[2,1,8-*gra*]naphthacene, 504

Naphtho[2,1-*b*]fluoranthene, 470
 Naphtho[2,1-*j*]fluoranthene, 482
 Naphtho[2,3-*j*]fluoranthene, 474
 Naphtho[2,3-*k*]fluoranthene, 484
 Naphtho[8,1,2-*ghi*]chrysene, 494
 Pentaleno[1,2-*b*:4,5-*b'*]dinaphthalene, 366
 $C_{24}H_{16}$
 Tetraphenylene, 512
 $C_{25}H_{16}$
 1*H*-Benz[4,5]indeno[1,2-*l*]phenanthrene, 516
 1*H*-Benz[*g*]indeno[2,1-*a*]phenanthrene, 518
 1*H*-Indeno[1,2-*a*]triphenylene, 520
 4*H*-Dibenzo[*a,de*]naphthacene, 530
 5*H*-Indeno[2,1-*a*]chrysene, 524
 7*H*-Benz[5,6]indeno[1,2-*a*]phenanthrene, 526
 7*H*-Benz[5,6]indeno[2,1-*a*]phenanthrene, 528
 7*H*-Benzo[*de*]pentacene, 532
 9*H*-Benz[4,5]indeno[2,1-*c*]phenanthrene, 522
 9*H*-Benz[5,6]indeno[2,1-*c*]phenanthrene, 514
 $C_{26}H_{14}$
 Acenaphtho[1,2-*j*]fluoranthene, 536
 Acenaphtho[1,2-*k*]fluoranthene, 538
 Anthra[2,1,9,8-*opqra*]naphthacene, 562
 Benz[*def*]indeno[1,2,3-*hi*]chrysene, 544
 Benz[*def*]indeno[1,2,3-*qr*]chrysene, 542
 Benzo[*qr*]naphtho[3,2,1,8-*defg*]chrysene, 552
 Dibenzo[*a,ghi*]perylene, 548
 Dibenzo[*b,ghi*]perylene, 554
 Dibenzo[*b,pqr*]perylene, 556
 Dibenzo[*cd,lm*]perylene, 564
 Fluoreno[3,2,1,9-*defg*]chrysene, 540
 Indeno[1,2,3-*cd*]perylene, 546
 Naphtho[1,2,3,4-*ghi*]perylene, 550
 Naphtho[7,8,1,2,3-*pqrst*]pentaphene, 560
 Naphtho[8,1,2-*bcd*]perylene, 558
 Rubicene, 534
 $C_{26}H_{16}$
 Anthra[1,2-*a*]anthracene, 578
 Benzo[*a*]naphth[2,1-*j*]anthracene, 582
 Benzo[*a*]naphtho[1,2-*h*]anthracene, 606
 Benzo[*a*]pentacene, 626
 Benzo[*a*]pentaphene, 602
 Benzo[*a*]picene, 608
 Benzo[*b*]picene, 628
 Benzo[*c*]pentaphene, 622

Benzo[*c*]picene, 636
 Benzo[*f*]picene, 598
 Benzo[*h*]pentaphene, 586
 Benzo[*s*]picene, 600
 Dibenzo[*a,c*]naphthacene, 588
 Dibenzo[*a,c*]tetraphene, 596
 Dibenzo[*a,j*]naphthacene, 624
 Dibenzo[*a,l*]naphthacene, 618
 Dibenzo[*b,k*]chrysene, 634
 Dibenzo[*b,l*]chrysene, 616
 Dibenzo[*b,p*]chrysene, 592
 Dibenzo[*c,g*]chrysene, 584
 Dibenzo[*c,l*]chrysene, 610
 Dibenzo[*c,p*]chrysene, 576
 Dibenzo[*g,p*]chrysene, 570
 Hexacene, 638
 Hexaphene, 620
 Naphtho[1,2-*a*]naphthacene, 604
 Naphtho[1,2-*b*]chrysene, 632
 Naphtho[1,2-*b*]triphenylene, 590
 Naphtho[1,2-*c*]chrysene, 612
 Naphtho[1,2-*g*]chrysene, 574
 Naphtho[2,1-*a*]naphthacene, 630
 Naphtho[2,1-*b*]chrysene, 614
 Naphtho[2,1-*c*]chrysene, 580
 Naphtho[2,3-*c*]chrysene, 594
 Naphtho[2,3-*g*]chrysene, 570
 Phenanthro[3,4-*c*]phenanthrene, 566
 Phenanthro[4,3-*a*]anthracene, 572
 C₂₇H₁₆
 8*H*-Tribenzo[*a,cd,l*]pyrene, 640
 9*H*-Naphtho[1,2,3-*cd*]perylene, 642
 C₂₇H₁₈
 Truxene, 646
 C₂₈H₁₄
 Acenaphtho[1,2-*k*]cyclopenta[*cd*]fluoranthene, 648
 Benzo[*a*]coronene, 654
 Benzo[*cd*]naphtho[3,2,1,8-*pqra*]perylene, 652
 Benzo[*lmn*]naphtho[2,1,8-*qra*]perylene, 658
 Benzo[*pqr*]naphtho[8,1,2-*bcd*]perylene, 660
 Diindeno[1,2,3-*cd*:1',*d'*,3'-*jk*]pyrene, 646
 peri-Naphthacenonaphthacene, 664
 Phenanthro[1,10,9,8-*opqra*]perylene, 650
 Phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene, 662
 Phenanthro[5,4,3,2-*abcde*]perylene, 656

$C_{28}H_{16}$

Anthra[1,2-*a*]aceanthrylene, 668
Anthra[2,1,9-*gra*]naphthacene, 752
Anthra[2,1-*a*]aceanthrylene, 670
Benzo[*a*]naphtho[2,1,8-*hij*]naphthacene, 748
Benzo[*a*]naphtho[8,1,2-*cde*]naphthacene, 706
Benzo[*a*]naphtho[8,1,2-*lmn*]naphthacene, 744
Benzo[*b*]naphtho[8,1,2-*pqr*]chrysene, 710
Benzo[*c*]naphtho[8,1,2-*ghi*]chrysene, 690
Benzo[*de*]naphtho[3,2,1-*mn*]naphthacene, 686
Benzo[*fg*]naphtho[1,2,3-*op*]naphthacene, 676
Benzo[*mno*]naphtho[1,2-*c*]chrysene, 742
Benzo[*mno*]naphtho[2,1-*c*]chrysene, 688
Benzo[*p*]naphtho[1,8,7-*ghi*]chrysene, 678
Benzo[*vwx*]hexaphene, 746
Dibenzo[*a,f*]perylene, 680
Dibenzo[*a,j*]perylene, 698
Dibenzo[*a,n*]perylene, 684
Dibenzo[*a,o*]perylene, 672
Dibenzo[*a,pqr*]picene, 734
Dibenzo[*a,rst*]pentaphene, 720
Dibenzo[*b,tuv*]picene, 760
Dibenzo[*c,pqr*]picene, 756
Dibenzo[*c,rst*]pentaphene, 758
Dibenzo[*de,ij*]pentaphene, 724
Dibenzo[*de,kl*]pentaphene, 740
Dibenzo[*de,qr*]pentacene, 738
Dibenzo[*de,st*]pentacene, 730
Dibenzo[*de,uv*]pentacene, 714
Dibenzo[*de,uv*]pentaphene, 718
Dibenzo[*f,pqr*]picene, 708
Dibenzo[*fg,ij*]pentaphene, 728
Dibenzo[*fg,qr*]pentacene, 736
Dibenzo[*h,rst*]pentaphene, 696
Dibenzo[*pq,uv*]pentaphene, 716
Fluoreno[9,1-*ab*]triphenylene, 666
Naphtho[1,2,3,4-*rst*]pentaphene, 704
Naphtho[1,2-*b*]perylene, 702
Naphtho[2,1,8-*def*]picene, 726
Naphtho[2,1,8-*fgh*]pentaphene, 700
Naphtho[2,1,8-*uva*]pentacene, 750
Naphtho[2,1,8-*uva*]pentaphene, 722
Naphtho[2,1-*b*]perylene, 732
Naphtho[8,1,2-*cde*]pentaphene, 754
Phenanthro[1,2,3,4-*def*]chrysene, 674

Phenanthro[9,10,1-*gra*]naphthacene, 694
 Tribenzo[*a,hi,mn*]naphthacene, 712
 Tribenzo[*b,def,p*]chrysene, 692
 Tribenzo[*c,g,mno*]chrysene, 682
 C₂₉H₁₈
 1*H*-Dibenzo[*a,de*]naphth[2,3-*h*]anthracene, 762
 4*H*-Dibenzo[*a,de*]pentacene, 764
 C₃₀H₁₄
 Dibenz[*e,ghi*]indeno[1,2,3,4-*pgra*]perylene, 768
 Dibenzo[*bc,ef*]coronene, 774
 Dibenzo[*bc,kl*]coronene, 776
 Dibenzo[*mn,qr*]fluoreno[2,1,9,8,7-*defghi*]naphthacene, 770
 Dicyclopenta[*a,j*]coronene, 766
 Naphtho[8,1,2-*abc*]coronene, 774
 C₃₀H₁₆
 Anthra[2,1,9,8-*defgh*]pentaphene, 822
 Anthra[2,1,9,8-*stuva*]pentacene, 874
 Anthra[8,9,1,2-*cdefg*]benzo[*a*]naphthacene, 828
 Anthra[8,9,1,2-*lmnop*]benzo[*a*]naphthacene, 870
 Anthra[9,1,2-*bcd*]perylene, 800
 Benzo[*a*]naphtho[1,2,3,4-*ghi*]perylene, 816
 Benzo[*a*]naphtho[2,1,8-*cde*]perylene, 784
 Benzo[*a*]naphtho[2,1,8-*lmn*]perylene, 796
 Benzo[*a*]naphtho[7,8,1,2,3-*pqrst*]pentaphene, 838
 Benzo[*a*]naphtho[8,1,2-*klm*]perylene, 802
 Benzo[*b*]naphtho[1,2,3,4-*pqr*]perylene, 788
 Benzo[*c*]naphtho[7,8,1,2,3-*pqrst*]pentaphene, 862
 Benzo[*de*]naphtho[2,1,8,7-*qrst*]pentacene, 854
 Benzo[*de*]naphtho[8,1,2,3-*stuv*]picene, 830
 Benzo[*ghi*]naphtho[2,1-*a*]perylene, 824
 Benzo[*ghi*]naphtho[2,1-*b*]perylene, 832
 Benzo[*h*]naphtho[7,8,1,2,3-*pqrst*]pentaphene, 792
 Benzo[*ij*]naphtho[2,1,8,7-*defg*]pentaphene, 850
 Benzo[*kl*]naphtho[2,1,8,7-*defg*]pentaphene, 848
 Benzo[*lm*]naphtho[1,8-*ab*]perylene, 812
 Benzo[*pqr*]naphtho[1,2-*b*]perylene, 810
 Benzo[*pqr*]naphtho[2,1,8-*def*]picene, 836
 Benzo[*pqr*]naphtho[2,1-*b*]perylene, 844
 Benzo[*pqr*]naphtho[8,1,2-*cde*]picene, 878
 Benzo[*qr*]naphtho[2,1,8,7-*defg*]pentacene, 856
 Benzo[*qr*]naphtho[2,1,8,7-*fghi*]pentacene, 842
 Benzo[*rst*]naphtho[2,1,8-*fgh*]pentaphene, 814
 Benzo[*rst*]naphtho[8,1,2-*cde*]pentaphene, 880
 Benzo[*st*]naphtho[2,1,8,7-*defg*]pentacene, 840
 Benzo[*uv*]naphtho[2,1,8,7-*defg*]pentacene, 834

Benzo[*uv*]naphtho[2,1,8,7-*defg*]pentaphene, 818
 Dibenzo[*b,qr*]naphtho[3,2,1,8-*defg*]chrysene, 826
 Dibenzo[*c,hi*]naphtho[3,2,1,8-*mno*]chrysene, 786
 Dibenzo[*de,mn*]naphtho[2,1,8-*qra*]naphthacene, 804
 Dinaphtho[8,1,2-*lmn*:2',1',8'-*qra*]naphthacene, 872
 Naphth[1',2':5,6]indeno[1,2,3-*cd*]pyrene, 778
 Naphth[2',1':4,5]indeno[1,2,3-*cd*]pyrene, 782
 Naphthaceno[2,1,12,11-*opqra*]naphthacene, 876
 Naphtho[3,2,1,8,7-*vwxyz*]hexaphene, 858
 Naphtho[7,8,1,2,3-*tuvwx*]hexaphene, 866
 Phenanthro[1,2,3,4-*ghi*]perylene, 808
 Phenanthro[2,3,4,5-*tuvab*]picene, 864
 Phenanthro[9,10,1,2,3-*pqrst*]pentaphene, 794
 Pyranthrene, 860
 Tetrabenzo[*de,hi,mn,qr*]naphthacene, 798
 Tribenzo[*a,cd,lm*]perylene, 808
 Tribenzo[*a,e,ghi*]perylene, 782
 Tribenzo[*a,ghi,k*]perylene, 820
 Tribenzo[*b,e,ghi*]perylene, 790
 Tribenzo[*b,n,pqr*]perylene, 846
 Tribenzo[*de,ij,rst*]pentaphene, 852
 Tribenzo[*de,kl,rst*]pentaphene, 868

$C_{30}H_{18}$

Anthra[1,2-*a*]benz[*j*]anthracene, 890
 Anthra[1,2-*a*]naphthacene, 918
 Anthra[2,1-*a*]naphthacene, 1058
 Benzo[2,1-*a*:3,4-*a'*]dianthracene, 884
 Benzo[*a*]hexacene, 1050
 Benzo[*a*]hexaphene, 966
 Benzo[*a*]naphtho[1,2-*c*]naphthacene, 960
 Benzo[*a*]naphtho[1,2-*j*]naphthacene, 1000
 Benzo[*a*]naphtho[1,2-*l*]naphthacene, 1024
 Benzo[*a*]naphtho[2,1-*j*]naphthacene, 1052
 Benzo[*a*]naphtho[2,1-*l*]naphthacene, 936
 Benzo[*b*]naphtho[1,2-*k*]chrysene, 1060
 Benzo[*b*]naphtho[1,2-*l*]chrysene, 1022
 Benzo[*b*]naphtho[2,1-*g*]chrysene, 922
 Benzo[*b*]naphtho[2,1-*k*]chrysene, 1028
 Benzo[*b*]naphtho[2,1-*p*]chrysene, 904
 Benzo[*b*]naphtho[2,3-*g*]chrysene, 902
 Benzo[*b*]naphtho[2,3-*l*]chrysene, 982
 Benzo[*c*]hexaphene, 1036
 Benzo[*c*]naphtho[1,2-*l*]chrysene, 1014
 Benzo[*c*]naphtho[2,1-*p*]chrysene, 882
 Benzo[*c*]naphtho[2,3-*l*]chrysene, 978

Benzo[*g*]naphtho[2,1-*b*]chrysene, 944
Benzo[*l*]naphtho[1,2-*b*]chrysene, 1012
Benzo[*l*]naphtho[2,1-*b*]chrysene, 1016
Benzo[*o*]hexaphene, 1034
Benzo[*p*]hexaphene, 1020
Benzo[*p*]naphtho[1,2-*b*]chrysene, 964
Benzo[*p*]naphtho[2,1-*b*]chrysene, 962
Benzo[*q*]hexaphene, 976
Dibenzo[*a,c*]pentacene, 958
Dibenzo[*a,c*]pentaphene, 954
Dibenzo[*a,c*]picene, 992
Dibenzo[*a,f*]picene, 918
Dibenzo[*a,h*]pentaphene, 902
Dibenzo[*a,j*]picene, 934
Dibenzo[*a,l*]pentacene, 1042
Dibenzo[*a,m*]pentaphene, 996
Dibenzo[*a,n*]pentacene, 1026
Dibenzo[*a,n*]picene, 1004
Dibenzo[*a,o*]pentaphene, 926
Dibenzo[*a,o*]picene, 952
Dibenzo[*b,f*]picene, 956
Dibenzo[*b,j*]picene, 982
Dibenzo[*b,m*]picene, 1056
Dibenzo[*b,n*]picene, 1040
Dibenzo[*b,s*]picene, 986
Dibenzo[*c,h*]pentaphene, 948
Dibenzo[*c,m*]pentaphene, 1046
Dibenzo[*c,m*]picene, 1064
Dibenzo[*c,s*]picene, 994
Dibenzo[*f,j*]picene, 946
Dibenzo[*f,s*]picene, 910
Dinaphth[1,2-*a*:1',2'-*h*]anthracene, 976
Dinaphth[1,2-*a*:2',1'-*j*]anthracene, 898
Dinaphtho[2,1-*c* 1',2'-*g*]phenanthrene, 886
Heptacene, 1066
Heptaphene, 1018
Naphtho[1,2-*a*]pentacene, 984
Naphtho[1,2-*a*]pentaphene, 920
Naphtho[1,2-*b*]picene, 998
Naphtho[1,2-*c*]pentaphene, 1048
Naphtho[1,2-*f*]picene, 928
Naphtho[1,2-*h*]pentaphene, 892
Naphtho[2,1-*a*]pentaphene, 990
Naphtho[2,1-*a*]picene, 1008
Naphtho[2,1-*b*]picene, 1054

Naphtho[2,1-*c*]pentaphene, 1008
 Naphtho[2,1-*c*]picene, 1010
 Naphtho[2,3-*a*]pentaphene, 942
 Naphtho[2,3-*a*]picene, 940
 Naphtho[2,3-*b*]picene, 1038
 Naphtho[2,3-*c*]pentaphene, 1044
 Naphtho[2,3-*s*]picene, 896
 Phenanthro[1,2-*a*]naphthacene, 968
 Phenanthro[1,2-*b*]chrysene, 1062
 Phenanthro[2,1-*b*]chrysene, 1030
 Phenanthro[2,3-*c*]chrysene, 924
 Phenanthro[2,3-*g*]chrysene, 914
 Phenanthro[3,2-*g*]chrysene, 896
 Phenanthro[3,4-*a*]naphthacene, 1032
 Phenanthro[3,4-*b*]chrysene, 942
 Phenanthro[3,4-*b*]triphenylene, 930
 Phenanthro[3,4-*c*]chrysene, 912
 Phenanthro[4,3-*b*]chrysene, 1002
 Phenanthro[9,10-*a*]naphthacene, 990
 Phenanthro[9,10-*b*]chrysene, 970
 Phenanthro[9,10-*b*]triphenylene, 906
 Tribenzo[*a,c,j*]naphthacene, 952
 Tribenzo[*b,g,k*]chrysene, 972
 Tribenzo[*b,g,l*]chrysene, 934
 Tribenzo[*b,g,p*]chrysene, 908
 Trinaphthylene, 890

$C_{32}H_{14}$

Ovalene, 1068

$C_{32}H_{16}$

Anthra[2,1,9,8,7-*defghi*]benzo[*op*]pentacene, 1138
 Anthra[2,1,9,8,7-*defghi*]benzo[*st*]pentacene, 1124
 Anthra[2,1,9,8,7-*defghi*]benzo[*uv*]pentacene, 1128
 Anthra[2,1,9,8-*defgh*]benzo[*rst*]pentaphene, 1106
 Anthra[3,2,1,9,8-*rstuva*]benzo[*ij*]pentaphene, 1118
 Anthra[3,2,1,9-*pqra*]benzo[*cd*]perylene, 1094
 Anthra[7,8,9,1,2,3-*rstuvw*]hexaphene, 1142
 Benzo[3,4]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene, 1094
 Benzo[*def*]pyranthrene, 1144
 Benzo[*e*]phenanthro[1,10,9,8-*opqra*]perylene, 1090
 Benzo[*e*]phenanthro[2,3,4,5-*pqrab*]perylene, 1074
 Benzo[*h*]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene, 1082
 Benzo[*lm*]phenanthro[5,4,3-*abcd*]perylene, 1114
 Dibenzo[*a,cd*]naphtho[8,1,2,3-*fghi*]perylene, 1072
 Dibenzo[*a,d*]coronene, 1080
 Dibenzo[*a,g*]coronene, 1110

Dibenz[*a,ghi*]naphtho[2,1,8-*cde*]perylene, 1070
 Dibenz[*a,ghi*]naphtho[2,1,8-*lmn*]perylene, 1078
 Dibenz[*a,ghi*]naphtho[8,1,2-*klm*]perylene, 1096
 Dibenz[*a,j*]coronene, 1126
 Dibenz[*cd,k*]naphtho[3,2,1,8-*pqra*]perylene, 1100
 Dibenz[*cd,n*]naphtho[3,2,1,8-*pqra*]perylene, 1108
 Dibenz[*de,ij*]naphtho[3,2,1,8,7-*rstuv*]pentaphene, 1120
 Dibenz[*de,ij*]naphtho[7,8,1,2,3-*pqrst*]pentaphene, 1116
 Dibenz[*fg,ij*]naphtho[7,8,1,2,3-*pqrst*]pentaphene, 1104
 Dibenz[*ghi,lm*]naphtho[1,8-*ab*]perylene, 1098
 Dibenz[*ghi,n*]naphtho[8,1,2-*bcd*]perylene, 1112
 Dibenz[*ij,rst*]naphtho[2,1,8,7-*defg*]pentaphene, 1132
 Dibenz[*kl,rst*]naphtho[2,1,8,7-*defg*]pentaphene, 1136
 Dinaphtho[1,8-*ab:8',1',2',3'-fghi*]perylene, 1076
 Dinaphtho[2,1,8,7-*defg:2',1',8',7'-ijkl*]pentaphene, 1134
 Dinaphtho[2,1,8,7-*defg:2',1',8',7'-opqr*]pentacene, 1140
 Dinaphtho[2,1,8,7-*defg:2',1',8',7'-qrst*]pentacene, 1130
 Dinaphtho[2,1,8-*fgh:3',2',1',8',7'-rstuv*]pentaphene, 1088
 Dinaphtho[2,1,8-*fgh:7',8',1',2',3'-pqrst*]pentaphene, 1084
 Dinaphtho[8,1,2-*cde:7',8',1',2',3'-pqrst*]pentaphene, 1148
 Naphtho[1,2-*a*]coronene, 1102
 Naphtho[2,3-*a*]coronene, 1122
 Phenanthro[2,1,10,9,8,7-*tuvwxyz*]hexaphene, 1146
 Pyreno[5,4,3,2,1-*pqrst*]pentaphene, 1086

C₃₂H₁₈

Anthra[1,2,3,4-*rst*]pentaphene, 1160
 Benzo[*h*]naphtho[1,2,3,4-*rst*]pentaphene, 1154
 Benzo[*tuv*]naphtho[2,1-*b*]picene, 1166
 Dibenz[*fg,st*]hexacene, 1162
 Dibenz[*q,vwx*]hexaphene, 1160
 Fluorantheno[8,9-*b*]triphenylene, 1150
 Naphtho[2,1,8-*yz*]hexacene, 1164
 Tetrabenz[*a,c,hi,mn*]naphthacene, 1156
 Tribenz[*a,f,j*]perylene, 1154

C₃₄H₁₆

Anthra[9,1,2-*abc*]coronene, 1182
 Benzo[*bc*]naphtho[1,2,3-*ef*]coronene, 1178
 Benzo[*bc*]naphtho[3,2,1-*ef*]coronene, 1172
 Benzo[*g*]naphtho[8,1,2-*abc*]coronene, 1176
 Benzo[*j*]naphtho[8,1,2-*abc*]coronene, 1192
 Benzo[*m*]naphtho[8,1,2-*abc*]coronene, 1188
 Benzo[*p*]naphtho[8,1,2-*abc*]coronene, 1168
 Benzo[*pqr*]dinaphtho[8,1,2-*bcd:2',1',8'-lmn*]perylene, 1194
 Dibenz[*fg,ij*]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene, 1184
 Naphtho[3,2,1,8,7-*defgh*]pyranthrene, 1196

peri-Pentacenopentacene, 1198
Perylo[3,2,1,12-*pqrab*]perylene, 1186
Phenanthro[10,1,2-*abc*]coronene, 1190
Tribenzo[*a,ef,hi*]coronene, 1174
Tribenzo[*a,ef,no*]coronene, 1172
Tribenzo[*a,hi,kl*]coronene, 1180

$C_{34}H_{18}$

Anthra[9,1,2-*cde*]benzo[*rst*]pentaphene, 1226
Benzo[*a*]pyranthrene, 1200
Benzo[*rst*]phenanthro[1,10,9-*cde*]pentaphene, 1220
Benzo[*rst*]phenanthro[10,1,2-*cde*]pentaphene, 1222
Dibenzo[*a,rst*]naphtho[8,1,2-*cde*]pentaphene, 1218
Dibenzo[*fg,ij*]naphtho[2,1,8-*uva*]pentaphene, 1210
Dibenzo[*fgh,pqr*]trinaphthylene, 1206
Dibenzo[*j,lm*]naphtho[1,8-*ab*]perylene, 1210
Dinaphtho[2,1,8-*jkl:2',1',8'-uva*]pentacene, 1226
Tetrabenzo[*a,cd,f,lm*]perylene, 1204
Tetrabenzo[*a,cd,j,lm*]perylene, 1208
Tetrabenzo[*de,h,kl,rst*]pentaphene, 1212
Tetrabenzo[*de,hi,op,st*]pentacene, 1216
Tetrabenzo[*de,jk,op,uv*]pentacene, 1214

$C_{34}H_{20}$

Benzo[6,7]phenanthro[4,3-*b*]chrysene, 1236
Benzo[*a*]heptacene, 1244
Benzo[*c*]naphtho[2,1-*m*]pentaphene, 1240
Benzo[*j*]benzo[2,1-*a:3,4-a'*]dianthracene, 1232
Dinaphtho[1,2-*b:1',2'-k*]chrysene, 1246
Dinaphtho[2,1-*a:1',2'-l*]naphthacene, 1238
Dinaphtho[2,1-*a:2',1'-j*]naphthacene, 1242
Naphtho[2,1-*c:7,8-c'*]diphenanthrene, 1228
Octacene, 1248
Phenanthro[2,1-*f*]picene, 1230
Tetrabenzo[*a,c,j,l*]naphthacene, 1234

$C_{36}H_{16}$

Anthra[1,9,8-*abcd*]benzo[*hi*]coronene, 1254
Benz[4,10]anthra[1,9,8-*abcd*]coronene, 1274
Benz[*a*]ovalene, 1268
Benz[*d*]ovalene, 1282
Benzo[*ef*]phenaleno[9,1,2-*abc*]coronene, 1258
Benzo[*qrs*]naphtho[3,2,1,8,7-*defgh*]pyranthrene, 1288
Dibenzo[*ef,hi*]naphtho[8,1,2-*abc*]coronene, 1264
Dibenzo[*ef,no*]naphtho[8,1,2-*abc*]coronene, 1252
Dibenzo[*hi,kl*]naphtho[8,1,2-*abc*]coronene, 1272
Dibenzo[*kl,no*]naphtho[8,1,2-*abc*]coronene, 1266
Dinaphtho[8,1,2-*abc:2',1',8'-efg*]coronene, 1262

Dinaphtho[8,1,2-*abc*:2',1',8'-*hij*]coronene, 1284
Dinaphtho[8,1,2-*abc*:2',1',8'-*klm*]coronene, 1278
Dinaphtho[8,1,2-*abc*:2',1',8'-*nop*]coronene, 1250
Dinaphtho[8,1,2-*abc*:8',1',2'-*ghi*]coronene, 1270
Dinaphtho[8,1,2-*abc*:8',1',2'-*jkl*]coronene, 1286
Pyreno[1,10,9-*abc*]coronene, 1276
Pyreno[10,1,2-*abc*]coronene, 1280
Tetrabenz[*bc,ef,hi,kl*]coronene, 1260
Tetrabenz[*bc,ef,kl,no*]coronene, 1256

$C_{36}H_{18}$

Anthra[2,3-*a*]coronene, 1305
Benzo[*rst*]dinaphtho[8,1,2-*cde*:2',1',8'-*klm*]pentaphene, 1309
Benzo[*rst*]pyreno[1,10,9-*cde*]pentaphene, 1303
Decacyclene, 1291
Dibenzo[*fg,ij*]phenanthro[9,10,1,2,3-*pqrst*]pentaphene, 1293
Dibenzo[*ij,rst*]phenanthro[9,10,1,2-*defg*]pentaphene, 1307
Dibenzo[*j,lm*]phenanthro[5,4,3-*abcd*]perylene, 1297
Dibenzo[*rs,vwx*]naphtho[2,1,8,7-*klmn*]hexaphene, 1301
Tribenzo[*fgh,pqr,za1b1*]trinaphthylene, 1295
Tribenzo[*jk,qr,uv*]naphtho[2,1,8,7-*defg*]pentacene, 1299

$C_{36}H_{20}$

Dibenzo[*b,tuv*]naphtho[2,1-*m*]picene, 1335
Dibenzo[*f,j*]naphtho[1,2,3,4-*pqr*]picene, 1321
Dinaphtho[1,2,3-*fg*:1',2',3'-*qr*]pentacene, 1327
Dinaphtho[1,2,3-*fg*:3',2',1'-*qr*]pentacene, 1321
Dinaphtho[1,2-*b,2',1'-n*]perylene, 1323
Dinaphtho[1,8-*bc*:1',8'-*mn*]picene, 1331
Dinaphtho[3,2,1-*fg*:1',2',3'-*ij*]pentaphene, 1325
Dinaphtho[3,2,1-*fg*:3',2',1'-*qr*]pentacene, 1317
Pyreno[2,1-*b*]picene, 1333
Tetrabenz[*a,c,hi,qr*]pentacene, 1329
Tetrabenz[*a,e,j,o*]perylene, 1313
Tetrabenz[*a,f,j,o*]perylene, 1317
Tetrabenz[*a,f,k,n*]perylene, 1311

$C_{38}H_{22}$

Chryseno[2,1-*b*]picene, 1343
Dinaphtho[2,3-*c*:2',3'-*m*]pentaphene, 1341
Diphenanthro[3,4-*c*:4',3'-*g*]phenanthrene, 1337
Nonacene, 1345
Tetrabenz[*a,c,l,n*]pentacene, 1339

Ceranthrene, 220

Cholanthrene, 172

Cholanthrylene, 150

Chrysene, 100

Chryseno[2,1-*b*]picene, 1343

Chrysofluorene, 80
Corannulene, 128
Coronene, 340
Cyclohexatriene, 16
Cyclopent[*b*]indeno[4,5-*g*]phenanthrene, 342
Cyclopent[*b*]indeno[5,6-*g*]phenanthrene, 344
Cyclopent[*i*]indeno[5,6-*a*]anthracene, 350
Cyclopenta[*cd*]perylene, 242
Cyclopenta[*cd*]pyrene, 86
Cyclopenta[*de*]anthracene, 60
Cyclopenta[*de*]naphthacene, 154
Cyclopenta[*de*]naphthalene, 34
Cyclopenta[*de*]pentacene, 442
Cyclopenta[*de*]pentaphene, 426
Cyclopenta[*de*]picene, 432
Cyclopenta[*fg*]naphthacene, 156
Cyclopenta[*fg*]pentacene, 440
Cyclopenta[*fg*]pentaphene, 406
Cyclopenta[*hi*]chrysene, 148
Cyclopenta[*jk*]phenanthrene, 58
Cyclopenta[*pq*]pentaphene, 408
Cyclopentaphenanthrene, 54

Decaylene, 1291
Dehydro-8,9-trimethylene-1,2-benzanthracene, 230
Di- β -naphthofluorene, 214
Dibenz[*a,c*]anthracene, 268
Dibenz[*a,e*]aceanthrylene, 450
Dibenz[*a,e*]acephenanthrylene, 446
Dibenz[*a,h*]anthracene, 282
Dibenz[*a,j*]aceanthrylene, 466
Dibenz[*a,j*]anthracene, 276
Dibenz[*a,k*]acephenanthrylene, 388
Dibenz[*a,l*]aceanthrylene, 452
Dibenz[*a,n*]triphenylene, 570
Dibenz[*de,kl*]anthracene, 168
Dibenz[*e,ghi*]indeno[1,2,3,4-*pqra*]perylene, 768
Dibenz[*e,j*]aceanthrylene, 398
Dibenz[*e,k*]acephenanthrylene, 478
Dibenz[*e,l*]aceanthrylene, 412
Dibenz[*e,l*]acephenanthrylene, 470
Dibenzo-1,2,7,8-anthracene, 276
Dibenzo-2,3,11,12-fluoranthene, 472
Dibenzo[*a,c*]chrysene, 598
Dibenzo[*a,c*]naphthacene, 588

Dibenzo[*a,c*]pentacene, 958
Dibenzo[*a,c*]pentaphene, 954
Dibenzo[*a,c*]picene, 992
Dibenzo[*a,c*]tetraphene, 596
Dibenzo[*a,c*]triphenylene, 570
Dibenzo[*a,cd*]naphtho[8,1,2,3-*fghi*]perylene, 1072
Dibenzo[*a,d*]coronene, 1080
Dibenzo[*a,e*]fluoranthene, 450
Dibenzo[*a,e*]pyrene, 490
Dibenzo[*a,f*]fluoranthene, 454
Dibenzo[*a,f*]perylene, 680
Dibenzo[*a,f*]picene, 918
Dibenzo[*a,f*]tetraphene, 570
Dibenzo[*a,g*]coronene, 1110
Dibenzo[*a,ghi*]naphtho[2,1,8-*cde*]perylene, 1070
Dibenzo[*a,ghi*]naphtho[2,1,8-*lmn*]perylene, 1078
Dibenzo[*a,ghi*]naphtho[8,1,2-*klm*]perylene, 1096
Dibenzo[*a,ghi*]perylene, 548
Dibenzo[*a,h*]pentaphene, 902
Dibenzo[*a,h*]phenanthrene, 284
Dibenzo[*a,h*]pyrene, 510
Dibenzo[*a,i*]pyrene, 508
Dibenzo[*a,j*]coronene, 1126
Dibenzo[*a,j*]fluoranthene, 464
Dibenzo[*a,j*]naphthacene, 624
Dibenzo[*a,j*]perylene, 698
Dibenzo[*a,j*]picene, 934
Dibenzo[*a,j*]tetracene, 624
Dibenzo[*a,jk*]fluorene, 162
Dibenzo[*a,k*]fluoranthene, 456
Dibenzo[*a,k*]tetraphene, 606
Dibenzo[*a,l*]fluoranthene, 444
Dibenzo[*a,l*]naphthacene, 618
Dibenzo[*a,l*]pentacene, 1042
Dibenzo[*a,l*]pyrene, 486
Dibenzo[*a,m*]pentaphene, 996
Dibenzo[*a,m*]tetraphene, 582
Dibenzo[*a,n*]pentacene, 1026
Dibenzo[*a,n*]perylene, 684
Dibenzo[*a,n*]picene, 1004
Dibenzo[*a,o*]pentaphene, 926
Dibenzo[*a,o*]perylene, 672
Dibenzo[*a,o*]picene, 952
Dibenzo[*a,p*]chrysene, 600
Dibenzo[*a,pqr*]picene, 734

Dibenzo[*a,rst*]naphtho[8,1,2-*cde*]pentaphene, 1218
Dibenzo[*a,rst*]pentaphene, 720
Dibenzo[*b,def*]chrysene, 510
Dibenzo[*b,e*]fluoranthene, 446
Dibenzo[*b,f*]picene, 956
Dibenzo[*b,g*]chrysene, 596
Dibenzo[*b,g*]phenanthrene, 272
Dibenzo[*b,ghi*]fluoranthene, 260
Dibenzo[*b,ghi*]perylene, 554
Dibenzo[*b,h*]phenanthrene, 278
Dibenzo[*b,h*]pyrene, 508
Dibenzo[*b,j*]fluoranthene, 476
Dibenzo[*b,j*]picene, 982
Dibenzo[*b,jk*]fluorene, 164
Dibenzo[*b,k*]chrysene, 634
Dibenzo[*b,k*]fluoranthene, 472
Dibenzo[*b,k*]perylene, 736
Dibenzo[*b,l*]chrysene, 616
Dibenzo[*b,l*]fluoranthene, 462
Dibenzo[*b,m*]picene, 1056
Dibenzo[*b,mno*]fluoranthene, 258
Dibenzo[*b,n*]pentaphene, 1018
Dibenzo[*b,n*]perylene, 728
Dibenzo[*b,n*]picene, 1040
Dibenzo[*b,p*]chrysene, 592
Dibenzo[*b,pqr*]perylene, 556
Dibenzo[*b,qr*]naphtho[3,2,1,8-*defg*]chrysene, 826
Dibenzo[*b,s*]picene, 986
Dibenzo[*b,tuv*]naphtho[2,1-*m*]picene, 1335
Dibenzo[*b,tuv*]picene, 760
Dibenzo[*bc,ef*]coronene, 774
Dibenzo[*bc,kl*]coronene, 776
Dibenzo[*c,f*]tetraphene, 592
Dibenzo[*c,g*]chrysene, 584
Dibenzo[*c,g*]phenanthrene, 266
Dibenzo[*c,h*]pentaphene, 948
Dibenzo[*c,hi*]naphtho[3,2,1,8-*mno*]chrysene, 786
Dibenzo[*c,i*]cyclopenta[*a*]fluorene, 346
Dibenzo[*c,k*]tetraphene, 632
Dibenzo[*c,l*]chrysene, 610
Dibenzo[*c,lm*]fluorene, 158
Dibenzo[*c,m*]pentaphene, 1046
Dibenzo[*c,m*]picene, 1064
Dibenzo[*c,m*]tetraphene, 614
Dibenzo[*c,mno*]chrysene, 500

Dibenzo[*c,p*]chrysene, 576
Dibenzo[*c,pqr*]picene, 756
Dibenzo[*c,rst*]pentaphene, 758
Dibenzo[*c,s*]picene, 994
Dibenzo[*cd,fg*]anthanthrene, 656
Dibenzo[*cd,hi*]anthanthrene, 658
Dibenzo[*cd,jk*]pyrene, 264
Dibenzo[*cd,k*]naphtho[3,2,1,8-*pqra*]perylene, 1100
Dibenzo[*cd,lm*]anthanthrene, 664
Dibenzo[*cd,lm*]perylene, 564
Dibenzo[*cd,n*]naphtho[3,2,1,8-*pqra*]perylene, 1108
Dibenzo[*de,ij*]naphtho[3,2,1,8,7-*rstuv*]pentaphene, 1120
Dibenzo[*de,ij*]naphtho[7,8,1,2,3-*pqrst*]pentaphene, 1116
Dibenzo[*de,ij*]pentaphene, 724
Dibenzo[*de,kl*]pentaphene, 740
Dibenzo[*de,mn*]naphthacene, 502
Dibenzo[*de,mn*]naphtho[2,1,8-*qra*]naphthacene, 804
Dibenzo[*de,op*]naphthacene, 498
Dibenzo[*de,qr*]naphthacene, 492
Dibenzo[*de,qr*]pentacene, 738
Dibenzo[*de,qr*]tetracene, 492
Dibenzo[*de,st*]pentacene, 730
Dibenzo[*de,uv*]pentacene, 714
Dibenzo[*de,uv*]pentaphene, 718
Dibenzo[*def,mno*]chrysene, 264
Dibenzo[*def,mno*]cyclopenta[*hi*]chrysene, 334
Dibenzo[*def,p*]chrysene, 486
Dibenzo[*e,ghi*]perylene, 556
Dibenzo[*e,l*]pyrene, 496
Dibenzo[*ef,hi*]naphtho[8,1,2-*abc*]coronene, 1264
Dibenzo[*ef,no*]naphtho[8,1,2-*abc*]coronene, 1252
Dibenzo[*f,j*]naphtho[1,2,3,4-*pqr*]picene, 1321
Dibenzo[*f,j*]picene, 946
Dibenzo[*f,m*]tetraphene, 590
Dibenzo[*f,pqr*]picene, 708
Dibenzo[*f,s*]picene, 910
Dibenzo[*fg,ij*]naphtho[2,1,8-*uva*]pentaphene, 1210
Dibenzo[*fg,ij*]naphtho[7,8,1,2,3-*pqrst*]pentaphene, 1104
Dibenzo[*fg,ij*]pentaphene, 728
Dibenzo[*fg,ij*]phenanthro[2,1,10,9,8,7-*pqrstuv*]pentaphene, 1184
Dibenzo[*fg,ij*]phenanthro[9,10,1,2,3-*pqrst*]pentaphene, 1293
Dibenzo[*fg,op*]anthanthrene, 650
Dibenzo[*fg,op*]naphthacene, 496
Dibenzo[*fg,qr*]pentacene, 736
Dibenzo[*fg,st*]hexacene, 1162

Dibenzofgh,pqr]trinaphthylene, 1206
 Dibenzog,p]chrysene, 570
 Dibenzoghi,lm]naphtho[1,8-ab]perylene, 1098
 Dibenzoghi,mno]fluoranthene, 128
 Dibenzoghi,n]naphtho[8,1,2-bcd]perylene, 1112
 Dibenzoghi,pqr]perylene, 340
 Dibenzoh,rst]pentaphene, 696
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